8:36AM A1.00002 Scanning tunneling microscopy and spectroscopy of graphene on graphite\(^1\), GUOHONG LI, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854 — Graphene, a single atomic layer of crystalline carbon, exhibits fascinating electronic properties owing to low energy quasiparticles that resemble relativistic Dirac fermions. Recent experiments on graphene deposited on insulating substrates revealed that substrate-induced potential fluctuations obscure the Dirac fermion nature of the carriers. Using low temperature scanning tunneling microscopy (STM) and spectroscopy (STS) we demonstrated that substrate-induced potential fluctuations are substantially reduced when graphene is deposited on graphite and that in these samples the intrinsic structural and electronic properties of graphene become accessible. We observed the honeycomb structure and the V-shaped density of states that vanishes at the Dirac point, characteristic of Dirac fermions. In finite magnetic field we observed the appearance of a single sequence of Landau levels, with square root dependence on level index and field, further attesting to the Dirac fermion nature of the charge carriers. The experiments give access to the fundamental parameters of the electronic spectrum in graphene including the Fermi velocity, electron-phonon coupling constant and electron-electron interactions. In addition they revealed the appearance of a small gap at the Dirac point and an anomaly at the Fermi energy. Work in collaboration with E.Y. Andrei and A. Luican.

\[1\] Work supported by DE-FG02-99ER45742 and NSF-DMR-0456473.

9:12AM A1.00003 Tuning the properties of Dirac fermions in graphene\(^1\), ALESSANDRA LANZARA, University California, Berkeley — Graphene, a one atom thick layer of carbon, the supposedly ideal Dirac material, has been under the radar of theorists and experimentalist for many decades. Although novel physical properties were envisioned, graphene, as any other 2D material, was presumed not to exist in its free state because of long wavelength fluctuations that easily destroy purely 2D membranes. The recent success in isolating a single sheet of graphene has certainly challenged this view. In this talk I will present our experimental work in this field using a combination of spectroscopic and microscopy tools. I’ll present experimental evidence of what drives the stability of a graphene membrane and show comparison between exfoliated and epitaxial graphene. I will then discuss the nature of fermions in graphene sheets and how their peculiar electronic structure can be tuned by engineering small terraces of graphene down to nm size, where the physics gets dominated by quantum confinement. The implications of our study on the properties of Dirac materials and their potential role for applications are discussed.

9:48AM A1.00004 The infrared conductivity of graphene\(^1\), ANTONIO CASTRO NETO, Boston University — The discovery of graphene is probably one of the most important events in modern condensed matter physics. Besides being a material that is only one atom thick, it has electronic properties which are usual when compared with ordinary metals and semiconductors. These unusual properties are reflected in its infrared conductivity. We will discuss the physical processes that affect the low frequency conductivity of graphene. We show that while the standard model of graphene is capable of explaining most of the features, it also fails in some aspects, indicating that we still do not have a full understanding of the physical mechanisms that control the electronic properties of this amazing material.

8:00AM A2.00001 Infrared spectroscopy of gated structures based on single- and bi-layer graphene\(^1\) DMITRI BASOV, UCSD — Infrared spectroscopy was employed to investigated the charge dynamics in graphene integrated in tunable gated devices (Nature Physics 4, 532 (2008)). These measurements verified that electrons in single-layer graphene behave like Dirac quasiparticles but most importantly revealed several unexpected results that are beyond the theoretical predictions for idealized graphene. Several of our findings including, a systematic enhancement of the Fermi velocity at low energy and also the “residual” conductivity at frequencies below 2EF are indicative of many-body interactions. Recent infrared study of bilayer graphene uncovered a pronounced asymmetry in the optical conductivity upon injection of electrons and holes (arXiv:0807.3776). We believe this result is suggestive of a marked asymmetry between the valence and conduction bands in bilayer samples.

\[1\] Work at UCSD is supported by DOE

1Work performed in collaboration with Thilo Kopp

8:36AM A2.00002 Oxide Nanoelectronics On Demand\(^1\), JEREMY LEVY, University of Pittsburgh — Electronic confinement at nanoscale dimensions remains a central means of science and technology. I will demonstrate nanoscale lateral confinement of a quasi-two-dimensional electron gas at the LaAlO\(_3/\)SrTiO\(_3\) interface and show how it can be exploited to create a variety of electronic devices. Using a conducting AFM probe it is possible to create tunnel junctions and field-effect transistors (FETs) with feature sizes comparable to the diameter of a single-wall nanotube. These devices can be modified or erased without complex or irreversible lithographic procedures. This new, on-demand nanoelectronics platform has the potential for widespread technological application.

\[1\] Support from the National Science Foundation is gratefully acknowledged (DMR-0704022).
9:12AM A2.00003 Role of the surface in the interfacial metal-insulator transition in LaAlO$_3$/SrTiO$_3$¹, C. STEPHEN HELLBERG, Naval Research Lab — The observed metal-insulator transition in thin films of LaAlO$_3$ on SrTiO$_3$ depends critically on the film thickness: a reversible transition consistently works best with films 3 unit cells thick. Using first-principles density functional calculations, the role of the surface in the interfacial metal insulator transition will be examined. Water adsorsbs strongly to the surface, dissociating and causing an unusual striped reconstruction. The adsorbates allow the creation of wires and devices at the interface. The positively charged AFM removes OH adsorbates, changing the interface from insulating to metallic. The negatively charged AFM removes H adsorbates, reversing the process.


9:48AM A2.00004 Potential Barrier Lowering and Electrical Transport at the LaAlO$_3$/SrTiO$_3$ Interface, YURI SUZUKI, University of California, Berkeley — Interfacial phenomena form the basis for modern-day devices and continue to be an area of fundamental interest in condensed matter research. Advances in oxide thin film fabrication have enabled the synthesis of atomically precise oxide interfaces and hence have allowed for controlled investigation of interfacial phenomena in these materials. With the rich variety of functionalities exhibited by transition-metal oxides, a wide array of novel properties may be achieved at oxide heterointerfaces. An exemplary study is the discovery of metallicty at the interface of two band insulators, LaAlO$_3$ (LAO) and SrTiO$_3$ (STO), which has stimulated many subsequent experimental as well as theoretical studies. However, there is still intense debate on the origin of metallicty, specifically whether it arises from electronic reconstruction or oxygen vacancies. Using a combination of vertical transport measurements across and lateral transport measurements along the LAO/STO heterointerface, we demonstrate that significant potential barrier lowering and band bending are the cause of interfacial metallicity. Transport measurements across the heterointerface, indicate that barrier lowering and enhanced band bending extends over 2.5 nm into LAO as well as STO. We explain the origins of high-temperature carrier saturation, lower carrier concentration, and higher mobility in the sample with the thinnest LAO film on a STO substrate. Lateral transport results suggest that parasitic interface scattering centers limit the low-temperature lateral electron mobility of the metallic channel.

*In collaboration with Franklin Wong, Miaofang Chi, Rajesh Chopdekar, Brittany Nelson-Cheeseman and Nigel Browning.

10:24AM A2.00005 Modulation Doping of Electrons and Holes at Oxide Interfaces, HAROLD HWANG, University of Tokyo and Japan Science and Technology Agency — No abstract available.

Monday, March 16, 2009 8:00AM - 11:00AM Session A3 DCMP: Fe-based Superconductors: Pairing Symmetry 301/302

8:00AM A3.00001 Andreev reflection spectroscopy of iron-based superconductors, C.L. CHIEN, Johns Hopkins University — After a reign of over two decades by the cuprate superconductors, several new families of iron-based high-temperature superconductives have recently been discovered. Essential to a superconductor is the nature of the superconducting gap, its value, its structure, and its temperature dependence. Point contact Andreev reflection (PCAR) spectroscopy operating in the ballistic limit is one of few techniques that can quantitatively measure the gap of these new Fe-based superconductors and its temperature dependence. In SmFeAs$_1-y$F$_y$ (0.15 ≤ y ≤ 0.30), we have determined a single gap $2\Delta/k_BT_C \approx 3.5-3.6$ close to the BCS s-wave prediction and with a BCS-like temperature dependence. These results will be compared with various theoretical possibilities and those obtained by other measurements, such as ARPES and penetration depth. While the principles of the PCAR spectroscopy are well established, poor contact control and ballistic heating might lead to the appearance of spurious gaps and pseudogaps in PCAR measurements. In collaboration with T. Y. Chen, S. X. Huang and Z. Tesanovic at JHU and R. H. Liu and X. H. Chen at USTC.


8:36AM A3.00002 Pairing symmetry of iron-based superconductors revealed by ARPES, HONG DING, Institute of Physics, Chinese Academy of Sciences — The recent discovery of superconductivity in iron-arsenic compounds with a transition temperature ($T_c$) as high as 56 K ended the monopoly of copper oxides in the family of high-$T_c$ superconductors. In this talk I will report our angle-resolved photoemission observation of the superconducting gap, including its momentum, temperature, and Fermi surface (FS) dependence in single crystals Ba$_2$K$_4$Fe$_2$As$_2$ ($T_c = 37$ K). We found two nodeless and nearly isotropic superconducting gaps around their respective FS sheets: a large gap ($\Delta \sim 12$ meV) on the two small hole-like and electron-like FS sheets, and a small gap ($\sim 6$ meV) on the large hole-like FS. The isotropic pairing interactions are strongly orbital dependent, as the ratio $\Delta_1/\Delta_2$ switches from weak to strong coupling on different bands. In addition, we have observed a dispersion kink that is likely related to a spin mode. These results reveal the importance of inter-band interactions in the pairing mechanism, and support the anti-phase s-wave pairing symmetry in the Fe-based superconductors.

9:12AM A3.00003 Magnetic penetration depth of oxy-ferropnictide superconductors, ANTONY CARRINGTON, University of Bristol — The determination of the symmetry of the superconducting order parameter is an important first step toward uncovering the mechanism of superconductivity in any material. In this regard, measurements of the magnetic penetration depth $\lambda$ have played an important role. Although not a true bulk probe, like specific heat, penetration depth measurements in the Meissner state probe a few thousand Angstroms below the crystal surface and so should be reasonably representative of the bulk. In this talk I will present data for the in-plane magnetic penetration depth of three different families of oxy-ferropnictide superconductors, measured on single crystals using a sensitive radio frequency tunnel diode oscillator technique. Our results for samples of SmFeAs$_1-y$F$_y$ (y ≤ 0.2) with $T_c \approx 45$ K show that $\lambda(T)$ has an exponential temperature dependence suggesting that the Fermi surface is fully gapped. However, data for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ ($T_c \approx 22$ K) show power-law behavior, $\Delta \lambda(T) \sim T^{1.7}$, at low temperature, possibly suggestive of line-nodes. Finally, data for LaFePO ($T_c \approx 6$ K) also show a power-law behavior for $\lambda(T)$, but in this case the temperature dependence is almost perfectly linear down to $T \approx 100$K. The results suggest that the gap symmetry may not be universal in all the oxy-ferropnictide superconductors.

9:48AM A3.00004 Antiferromagnetic Correlation and the Pairing Mechanism of the Cuprates and Iron Pnictides: A View From the Functional Renormalization Group Studies, DUNG-HAI LEE, U.C. Berkeley — We study the pairing symmetry of the iron pnictide superconductor using the functional renormalization group method. By comparing the results for the cuprates and the iron pnictides a coherent picture emerges. It suggests that antiferromagnetic correlation causes pairing for both materials. In collaboration with Fa Wang, Hui Zhai, Ying Ran, and Ashvin Vishwanath, University of California, Berkeley.

¹Work supported by DOE.
10:24AM A3.00005 Superconductivity, magnetism, and pairing symmetry in Fe-based superconductors\textsuperscript{1}.
ILYA EREMIN, Max-Planck Institute for Physics of Complex Systems, Dresden — We analyze antiferromagnetism and superconductivity within the renormalization group (RG) technique in novel Fe-based superconductors. We find that the T dependencies of the spin susceptibility and NMR relaxation rate for such state are exponential only at very low T, and can be well fitted by power-laws over a wide T range below Tc. We further show that below Tc excitonic resonance appears in the spin excitations spectrum.

\textsuperscript{1}Work done in collaboration with A.V. Chubukov, D. Efremov, and M.M. Korshunov

Monday, March 16, 2009 8:00AM - 11:00AM — Session A4 DPOLY: Polymers and Energy Applications

8:00AM A4.00001 Ion solvation and its effects on the miscibility of binary polymer blends.
ZHENGANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — We study the effects of adding salt ions on the miscibility of a binary blend of polymers having different dielectric constants. The competition between the preference of the ions to be solvated by the component of the higher dielectric constant and the entropic tendency for the ions to be distributed uniformly results in non-trivial effects on the miscibility. We first study the thermodynamics of the polymer blend-ion mixture using a simple Born model in a uniform dielectric medium of the average composition of the polymer blend. We then study the effect of local enrichment of the higher dielectric constant polymer near the ion. We find that when the dielectric constants of the polymers are both low, adding salt decreases the miscibility, while when the dielectric constants of the polymers are both high, the addition of salt enhances the miscibility. When the blend consists of a high dielectric constant polymer and a low dielectric constant polymer, miscibility is decreased if the low dielectric constant component is the majority and is increased if the high dielectric constant component is the majority. The effect becomes significant at ion concentrations corresponding to an order of one ion per polymer chain. The quantitative change in the effective $\chi$ parameter depends on the functional form of the composition dependence of the dielectric constant of the mixture. We also illustrate the difference between fixed ion concentration and fixed chemical potential of the ions.

8:36AM A4.00002 The Nanostructure of Nafion for Fuel-Cell Membranes from Small-Angle Scattering and NMR Analysis\textsuperscript{1}.
KLAUS SCHMIDT-ROHR, Ames Laboratory and Dept. of Chemistry, Iowa State University, Ames, IA 50011, USA — We have investigated the long contentious nanometer-scale structure of the Nafion ionomer used in proton exchange membranes of H$_2$/O$_2$ fuel cells. Using a simple algorithm based on 3D numerical Fourier transformation, we have quantitatively simulated previously published small-angle scattering data of hydrated Nafion. The characteristic "ionomer peak" arises from long, parallel but otherwise randomly packed water channels surrounded by the partially hydrophilic sidebranches, forming inverted-micelle cylinders. The channels are stabilized by the considerable stiffness of the Nafion backbones, detected by $^{13}$C and $^{19}$F NMR. An upper limit of 300 nm to the persistence length of the water channels has been estimated from $^{2}$H NMR of $^{2}$H$_2$O in the channels. At 20 vol% water, the water channels have diameters between 1.8 and 3.5 nm, with a 2.4-nm average. The hydration-induced changes in small-angle scattering patterns and in the surface-to-volume ratio have also been analyzed in quantitative detail. Nafion crystallites ($\sim$10 vol%), which form physical crosslinks crucial for the mechanical properties of Nafion films, are elongated and parallel to the water channels, with cross sections of $\sim$5 nm$^2$. Simulations for a dozen other models of Nafion, including Glarke’s cluster and the polymer-bundle model, do not match the scattering data. The water-channel model is the first without constraints of $\sim$1.2 nm diameter; it can explain important features of Nafion, including fast diffusion of water and protons through Nafion and its persistence at low temperatures.

\textsuperscript{1}This work was supported by the U.S. Department of Energy - Basic Energy Sciences under Contract No. DE-AC02-07CH11358

YUE-LIN LOO, Princeton University — Organic solar cells have been proposed as low-cost and sustainable alternatives for power generation. To realize the low cost aspects of organic solar cells, conventional vacuum deposition technologies are to be replaced with solution processing. Our group has focused on the development of solution processable conductive polymers. Conductive polymers, like polyaniline, are generally doped with small-molecule acids. Though highly conductive, such materials are not processable. To overcome this intractability, polymer-acid dopants have replaced small-molecule acids. While the introduction of polymer acids render the conductive polymer solution processable, such gains in processability are accompanied by reduced conductivities. With a post-processing solvent-annealing treatment, however, we have been able to dramatically improve the electrical properties of polymer-acid doped conductive polymers; these polymers make efficient anodes in organic solar cells. To further improve the efficiencies of organic solar cells, we have introduced fractional amounts of additives within the active layer of the device. Depending on the hydrophobicity of the additives, they preferentially segregate into the electron donor phase, effectively enhancing phase separation between the electron donor and electron acceptor. This change in morphology increases charge separation; we see a two-fold increase in the short-circuit current in such devices over those without additives in the active layer.

9:48AM A4.00004 Charge Transport and Storage within Radical Redox Polymers as Electroattractive Materials in Energy Devices.
HIROYUKI NISHIDE, Waseda University — No abstract available.

10:24AM A4.00005 Polymers as active components in harnessing solar energy.
JAYANT KUMAR, University of Massachusetts, Lowell — In the last couple of decades molecular and polymeric photovoltaic cells have attracted considerable attention as a possible low cost alternative to conventional semiconductor solar cells. While considerable advances in improving device efficiencies have been made, significant challenges in developing efficient, reliable and low cost solar cells using polymers as an active component remain. Some of these advances and challenges as well as ongoing efforts to mass manufacture solar cells modules will be discussed.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A5 FIAP: Nanostructuring with Ions

401/402
8:00AM A. VAN KAN, CIBA, Physics Dept, NUS — Proton beam writing (PBW) is a new direct write lithography using MeV protons, and is unique because of its ability to fabricate 3D structures of high aspect ratio structures directly in resist material like PMMA, SU-8 and HSQ. The introduction by CIBA, Singapore of a dedicated PBW facility, capable of writing at the micro- and nano-scale has facilitated high aspect ratio nanostructuring. PBW has demonstrated high aspect ratio walls in HSQ down to the 20nm level. In recent experiments details down to sub 20 nm have been achieved in PMMA. Monte-Carlo calculations have shown that structuring down to the nanometer level is feasible. All this is possible because of the virtual absence of proximity effects (unwanted resist exposure by stray secondary electrons). The design and performance of this unique nanopatterning facility will be discussed. Two potential fields of application (nanofluidics and nanowire integration) of PBW will be discussed. Currently nanofluidics devices have typically only one critical dimension below 100 nm. Here we will introduce PBW as a powerful technique to fabricate molds for replication of PDMS nanofluidic circuits down to the sub 100 nm level in two dimensions. Initial chips with dimension down to 150 nm have successfully been used to study DNA folding in quasi-1d nanochannels in tandem with fluorescence imaging. Since the size of these PDMS nanochannels is not limited by the PDMS or PBW further miniaturization down to the sub 100 nm level is a realistic goal and initial results will be discussed. Nanowires are a potential building block for nano-electronic devices, and one critical problem is the integration of nanowires to form contacts. Porous alumina templates and high energy ion-tracks have been used for the production of nanowire templates in a random orientation. Since PBW is the only true 3D direct write nanolithographic technique it can be used to fabricate nanowire templates in a controlled manner.


9:12AM ANDREAS DIRK WIECK, Ruhr-Universität Bochum, D-44780 Bochum — The maskless implantation of FBIs in semiconductors creates a local dop. In n-type conducting sheets, p-lines are written to insulate n-regions laterally from each other or vice versa. In this way, conducting areas can be biased with respect to each other. Narrow paths are easily driven into depletion, creating lateral transistor channels. The advent of multi-focused-ion-beams allows a more parallel writing of such integrated circuits. For ion beam milling, a new long-life Bismuth (Bi) source is developed and employed [1]. Bi is the heaviest, non-radioactive element and has thus a maximal impact on the material to be sputtered locally. It is non-toxic, well available, mono-isotopic, and inexpensive, has a low melting temperature, and comes even in clusters and the single charged particles make up 95% of the whole FIB-beam. This means that the chromatic errors of the electrostatic Einzel-lenses in the FIB system are not important. Since heavy ions are slower than light ones at the same energy, Bi penetrates to a minimal depth into the target, leaving minimal contaminations. The sputter rate is about 5 times higher than the one of the usual Ga. Since Bi is the only element in this source, it is not necessary to separate it from other ions by a mass filter. Bi is thus a good candidate to improve the performance of spatter-FBIs ultimately or replacing Ga. We developed FBIs liquid metal ion sources of nearly all application elements in the periodic table. In this way, practically all dopants can be introduced into semiconductors after epitaxial growth in a full ultra-high vacuum process, which enhances the flexibility of the material choice enormously.

9:48AM — The helium ion microscope (HeIM) is a new, powerful instrument for nano-meterology and nanotechnology. As an emerging imaging and measurement tool it offers several advantages over the traditional scanning electron microscope (SEM) currently in use in research and manufacturing facilities across the world. First, resolution 2 to 4 times better than that from comparable SEMs is theoretically possible, due to the very high source brightness and the short wavelength of the helium ions. Ion images with unprecedented resolution have been routinely obtained on a wide range of samples with sub-nanometer features. More importantly, the interaction volume of the helium ion beam in the sample is substantially different in its size and shape from that of the electron beam in an SEM. As a consequence, the signals generated, especially secondary electrons, reveal more surface details. Imaging by the HeIM can further benefit from the superb depth of field and the fact that He ion imaging is less susceptible to sample charging. In addition, it is possible to compensate for charging by the use of an electron flood gun. Scattered He ions produced as a result of Rutherford scattering of the incident ions on the target nuclei can provide material contrast information that can be used for quantitative compositional analysis. Beyond imaging, the HeIM is a potent tool for milling and modifying surface structures at the nanometer scale, due to the relatively low mass of the helium ion, the narrow ion beam, and especially the low beam currents. It is possible to drill close to 10 nm diameter holes and mill other nanoscale structures that cannot be fabricated with any other method. It is expected that, as with the electron beam, it is feasible to deposit and deposit various materials with He ion beam irradiation. The work is at its exploratory stage, and likely soon will yield more exciting results. This presentation will report on some of the newest research work on the NIST helium ion microscope. 

10:24AM JOHN MELNGAILIS, University of Maryland — Both focused ion beams and electron beams can be used for direct, maskless, resistless nanofabrication as well as for lithography. So far the direct fabrication has been limited to applications such as photomask repair, circuit restructuring, failure analysis, and the creation of various highly specialized structures. Recent developments in maskless fabrication, so far aimed mainly at to resist exposure, suggest that this picture might change. For example, IMS in Vienna, Austria is developing an instrument that can be characterized as an ion beam or electron beam dot matrix printer. The total current on the sample available from this kind of instrument is at least three orders of magnitude larger than from a single beam instrument. This may lead to new applications of charged particle beam fabrication, as well as enable applications considered in the past but rejected because of very low throughput. An example of one such application is the direct writing of the identity in RFID tags using ion beam implantation. Recently we have also shown that electron beams can be used to deposit relatively pure platinum from an inorganic precursor gas, Pt(PF3)4. Such metal deposits can be used as contacts to carbon nanotubes, semiconductor nano wires, organic fibers, or other structures where conventional lithography is impractical.

1Some of the material for this talk is provided by Hans Loeschner and Elmar Platggerummer from IMS Nanofabrication AG, Vienna Austria
circuits, which will allow us to discern the function of natural systems and aid us in engineering synthetic systems. We have endeavored to address the following two questions: What makes the Start transition irreversible? How does the cell pool resources to achieve this transition? This motivates our use of the budding yeast model organism, whose Start checkpoint integrates multiple internal (e.g., cell size) and external signals into an irreversible decision to enter the cell cycle. We have undertaken a systems biology approach to address these questions by applying the tools of computational and systems biology. In particular, we have used systems biology to develop a mathematical model to describe the cell cycle, and we have used this model to make predictions and test hypotheses. We have also used directed evolution to identify novel factors that affect the Start transition. We have found that Start is regulated by a complex network of interactions between multiple factors, and that the network is highly dynamic and responsive to changes in the environment. This work has provided new insights into the regulation of the cell cycle and the development of new strategies for controlling cell proliferation in disease. In addition, it has highlighted the role of systems biology in advancing our understanding of complex biological processes.
9:12AM A7.00003 Signal integration, gain, and integral feedback in the *Escherichia coli* chemotaxis network, NED WINGREEN, Princeton University — Bacteria are able to sense chemicals in their environment, allowing cells to swim towards nutrients (attractant chemicals) and away from repellents (toxic chemicals). The chemotaxis network of the model bacterium *Escherichia coli* possesses remarkable signaling properties including high sensitivity to small changes in chemical concentration over a wide range of ambient concentrations. These signaling properties rely on the architecture of the circuit, including elements that implement signal integration, gain, and integral feedback. All of these elements rely on receptor clustering, which occurs at multiple length scales. At a small scale, the chemotaxis receptors form stable homodimers which then assemble into a larger complex in which receptors of different chemical specificities are intermixed, with trimers of dimers believed to be the smallest signaling unit. At a larger scale, ~10,000 receptors form large polar and lateral receptor clusters. I will discuss recent experimental and theoretical progress in understanding how the biophysics of chemotaxis receptors leads to the remarkable signaling properties of the chemotaxis network.

9:48AM A7.00004 Dissecting the nitrogen assimilation system of *E. coli*: from molecules to physiology, TERRY HWA, U.C. San Diego — Nitrogen assimilation is a major branch of cellular metabolism. For enteric bacteria such as *E. coli*, all of the nitrogen groups needed in biosynthesis are converted from ammonia by a relatively simple system comprised of 3 enzymes and 3 intermediate metabolites. This system is intricately regulated, at both the transcriptional and post-translational levels according to the nitrogen and carbon/energy status of the cell. While specific pieces of this regulation have been known for a long time, the strategy of regulation relating nitrogen influx to cellular demand is poorly understood. Clearly, the paradigm of end-product feedback inhibition well-established for the regulation of individual metabolic pathways is inadequate since there are too many products involving nitrogen. Through extensive experimental studies including quantitative characterization of the levels of key metabolites and enzymes for a carefully chosen spectrum of growth conditions and mutants, we obtain a dynamic picture of how the cell matches its rate of nitrogen assimilation with physiological needs through the intermediate metabolites.

1This research is supported by the Human Frontiers in Science Program and by the NSF.

10:24AM A7.00005 Building a genetic transistor in yeast: How protein sequestration generates a tunable ultrasensitive or all-or-none response, NICOLAS BUCHLER, Rockefeller University — Protein sequestration, where an active protein (A) is bound in an inactive complex by an inhibitor, is a common molecular mechanism in natural regulatory circuits. The inhibitor serves as a molecular sink that can buffer and titrate low concentrations of A. If sufficient protein A is produced, then the sink is saturated and A will exhibit an ultrasensitive or all-or-none response. Theory demonstrates that this ultrasensitivity grows both as a function of inhibitor concentration and increased binding affinity. Although protein sequestration can theoretically generate tunable ultrasensitive responses, this regulatory principle has never been tested experimentally. We used a synthetic genetic circuit in budding yeast to show that sequestration of a basic leucine zipper transcription factor (C/EBPa) by a dominant-negative inhibitor converts a graded transcriptional response into an ultrasensitive response, with apparent Hill coefficients up to 12. We developed a simple quantitative model for this genetic network that demonstrates how the threshold and degree of ultrasensitivity depend upon the abundance of the inhibitor, exactly as observed in our experimental results. Many proteins in natural regulatory networks involve the formation of inactive protein-protein complexes, e.g. stoichiometric inhibitors of kinases and dominant-negative inhibitors of transcription factors. Our results demonstrate that protein sequestration can provide potent and tunable ultrasensitivity in genetic networks. Ultrasensitive or all-or-none responses are critical for robust bistable or oscillatory genetic networks, and our findings suggest that protein sequestration might play an unappreciated role in facilitating the evolution of bistable or oscillatory circuits in natural systems.

Monday, March 16, 2009 8:00AM - 11:00AM —
Session A8 GQI: Quantum Information meets Many-Particle Physics 414/415

8:00AM A8.00001 Preparing ground states of quantum many-body systems on a quantum computer, DAVID POULIN, Département de Physique, Université de Sherbrooke, QC, Canada — The simulation of quantum many-body systems is known algorithm to prepare the ground state of a classical many-body system on a quantum computer [3,2]. This provides strong evidence that for a quantum computer can naturally implement the dynamics of a quantum system — i.e. solve Schrödinger’s equation — there was until now no general method for a carefully chosen spectrum of growth conditions and mutants, we obtain a dynamic picture of how the cell matches its rate of nitrogen assimilation with physiological needs through the intermediate metabolites.

**References**


8:36AM A8.00002 Topological Quantum Order from Symmetry and the Role of Temperature, GERARDO ORTIZ, Indiana University — What does a fractional quantum Hall liquid and Kitaev’s proposals for topological quantum computation have in common? It turns out that they are physical systems that exhibit degenerate ground states with properties seemingly different than ordinary (Landau-type) phases of matter, such as ferromagnets. For example, those (topologically quantum ordered) states cannot be characterized by (local) order parameters such as magnetization. How does one characterize this new order? I will present a unifying framework which will allow us to engineer physical systems displaying topological quantum order. What are the physical properties of these new orders? How robust are they to temperature effects? What are they useful for? Topologically quantum ordered states of matter seem to be ideal physical systems to store and manipulate quantum information since they are believed to be robust against decoherence with an environment, and thus appropriate for building a quantum computer and quantum memories. I will discuss the role of temperature in the protection of quantum information. Have we finally found a new technological application for quantum Hall liquids?

1Work done in collaboration with Zohar Nussinov
9:12AM A8.00003 Tensor-entanglement renormalization. ZHENGCHENG GU, M.I.T. — Traditional mean-field theory is a simple generic variational approach for analyzing various symmetry breaking phases. However, this simple approach only applies to symmetry breaking states with short-range entanglement. Tensor-entanglement renormalization group (TERG) is a generic approach for studying 2D quantum phases with long-range entanglement (such as topological phases) based on a new class of trial wavefunctions - the tensor product states (TPS), also known as projected entangled pair states (PEPS). Those TPS (PEPS) are built from local tensors. They can describe both states with short-range entanglement (such as the symmetry breaking states) and states with long-range entanglement (such as topological/classical order). TERG is a real space renormalization group algorithm that can efficiently simulate expectation values for TPS wave functions in 2D and higher dimensions. As an attempt in this direction, we demonstrate our algorithm by studying several simple 2D quantum spin models, including both symmetry breaking phase transitions and topological phase transitions. However, as any variational method, the TERG approach could not find all the degenerate ground states for gapped systems and generally could not give out (approximately) correct critical exponent for critical systems. To solve these problems, we study the renormalization group flow of a Lagrangian (partition function) by representing its path integral through a tensor network. Using a tensor-entanglement-filtering renormalization group (TEFRG) method that removes local entanglement and coarse grains the lattice, we show that the renormalization flow of the tensors in the tensor network has a nice fixed-point structure. The isolated fixed-point tensors characterize various phases. The tensor fixed points can describe both the symmetry breaking phases and topological phases. The ground state degeneracy for gapped systems can be easily read out from the fixed point tensor. The scaling dimensions, the central charge and dynamic correlation functions for the critical systems that describe the continuous phase transitions between symmetry breaking and/or topological phases can also be calculated from the TEFRG approach.

9:48AM A8.00004 Can multi-particle systems be too entangled to be useful for quantum computation? JENS EISERT, Blackett Laboratory, Imperial College London — In the context of “quantum information meets many-particle physics”, we pose the question of the role of entanglement in the quantum computational power of many-particle quantum systems (1) and the magnitude of quantum fluctuations (2). Our results show that computational universality is actually a rare property in quantum states. For the proof we make use of a link between the quantum probabilistic method and ideas on quantum many-body systems. This work stresses a new aspect of the question concerning the role entanglement plays for quantum computational speed-ups. We will also investigate a new classification of primitives from projected entangled pair states (PEPS) that can be used in order to systematically construct new models for measurement-based computation (2,3) and demonstrate for example that computational efficiency is actually a rare property in quantum states.

1 Supported in part by ONR Grant No. N00014-07-1-0304 and NSF Grant No. PHY-0653596.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A9 GSNP: Systems Far from Equilibrium I 303

8:00AM A9.00001 Directed motion and useful work from an isotropic non-equilibrium distribution. DANIEL KOSOV, University of Maryland, MAXIM GELIN, TU Munich — Since the Maxwell demon thought experiment, the extraction of useful work and directed motion from unbiased non-equilibrium distributions has been the source of fascination, intrigue, and confusion. Being a fundamental scientific problem, it is also of significant practical interest for various biological and nanotechnological applications. We propose a new type of “motor” driven by the heat flow between non-equilibrium velocity and equilibrium coordinate distributions. Namely, we demonstrate that a gas of classical particles trapped in an external asymmetric potential undergoes a quasiperiodic motion, if the temperature of its initial velocity distribution Tne differs from the equilibrium temperature Teq. The “loading” and “unloading” of the gas particles change directions of their motion, thereby creating a possibility of shuttle-like motion. The system works as a Carnot engine where the heat flow between kinetic and potential parts of the non-equilibrium distribution produces the useful work. Phys.Rev. E 77, 011115 (2008)

8:12AM A9.00002 Coherent transport and heat, entropy fluctuations in a thermal Brownian motor. RONALD BENJAMIN, University of Alabama at Birmingham — We investigate the heat, entropy and work fluctuations in a thermal Brownian motor driven by spatially inhomogeneous temperature. We show that the total heat, entropy production and the work fluctuations satisfy the fluctuation theorem in the steady state over finite time trajectories. The transport coherence of the motor, as determined by the Peclet number is also investigated as a function of various parameters of the system.

1 I thank the University of Alabama, Birmingham Graduate school for GAFP Fellowship.
36: A00004 Rapidly forced quantum Brownian motion. MUSTANSIR BARMA, MALAY BANDYOPADHYAY, Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai 400005, India — We study the steady state behaviour of a confined quantum Brownian particle which is subjected to a space-dependent, rapidly oscillating time-periodic force. To leading order in the period of driving, the result of the oscillating force is to produce an effective static potential which has a quantum contribution $V_q$, which adds on to the classical result. This is shown by using a coherent state representation of bath oscillators which leads to a c-numbered generalized quantum Langevin equation. We evaluate $V_q$ exactly in the case of an Ohmic dissipation bath and show that it takes on different forms in different regimes, determined by the ratio of the thermal wavelength to the spatial spread of the driving force.

4: A00005 Deciding how far is far from equilibrium. ANTONIO CADILHE, ARTHUR VOTER, Theoretical Division, T-1, MS B268, Los Alamos National Laboratory, Los Alamos, NM 87545 — Nonequilibrium systems have both fundamental and technological interest for their unusual behavior with research efforts mainly focused on their properties. Surprisingly, little research effort has been put on diagnosing how far a system is from equilibrium. Clearly, addressing such an issue is of fundamental and technological relevance. To this end, we present results of how a particle in contact with a heat reservoir is being driven away from equilibrium by a time dependent potential well. The methodology can be straightforwardly extended to systems with the influence of under the more realistic potentialials. More particles and under the influence of more realistic potentialials.

8: A00006 Random Sequential Adsorption on patterned substrates: jammed state structure and kinetic properties N. A. M. ARAUJO, J. F. MARQUES, GCEP-Centro de Fisica da Universidade do Minho, Braga, Portugal, A. CARDILHE, GCEP-Centro de Fisica da Universidade do Minho, Braga, Portugal. T-1 Group, MS B268, Los Alamos National Laboratory, Los Alamos, NM, USA, V. PRIVMAN, Department of Physics, and Center for Advanced Materials Processing, Clarkson University, Potsdam, NY, USA — The irreversible adsorption on a patterned substrate is studied through extensive Monte Carlo simulations. As a pattern, we adopted square cells positioned at the vertices of a square lattice. Particles attempting adsorption can only stick to the substrate if they do not overlap previously adsorbed ones (excluded volume interaction) and if their geometrical centers land inside a cell. Once a particle is adsorbed, it does not detach from or diffuse on the substrate, thus representing an extended random sequential adsorption model. The distribution of particles sizes follows a truncated gaussian-size distribution with values of the size dispersion varying from zero (monodisperse) to 20% (polydisperse) of the mean particle radius. We address the influence of both the pattern and size dispersion on the jammed state structure. We also present results on how the kinetics of approach to the jammed state is affected by the particular values taken by parameters like cell size and cell-cell separation and show that they can lead to either exponential or power-law functional dependences.

8: A00007 Phase Transition with Non-Thermodynamic States in Reversible Polymerization, ELI BEN-NAIM, Los Alamos National Laboratory, PAUL KRAPIVSKY, Boston University — We investigate a reversible polymerization process in which individual polymers aggregate and fragment at a rate proportional to their molecular weight. We find a nonequilibrium phase transition despite the fact that the dynamics are perfectly reversible. When the strength of the fragmentation process exceeds a critical threshold, the system reaches a thermodynamic steady state where the total number of polymers is proportional to the system size. The polymer length distribution has a sharp exponential tail in this case. When the strength of the fragmentation process falls below the critical threshold, the steady state becomes non-thermodynamic as the total number of polymers grows sub-linearly with the system size. Moreover, the length distribution has an algebraic tail and the characteristic exponent varies continuously with the fragmentation rate.

8: A00008 Stochastic continuum theory of active nematics, SHRADHA MISHRA, Syracuse University, FRANCESCO GINELLI, HUGUES CHATE, CEA Service de Physique de l’Etat Condense, CEN Saclay, 91191 Gif-sur-Yvette, France, SANJAY PURI, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore, SIRIRAM RAMASWAMY, Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore, India — We derive a stochastic continuum theory of active nematics by direct coarse-graining of a generic microscopic model and study numerically. This allows to characterize the microscopic origin of the various terms found and to determine the non-trivial structure of the noises. We show in particular that two terms coupling density and order the non-equilibrium active current argued before to be at the origin of giant density fluctuations, and a multiplicative conserved noise are necessary to obtain a faithful description of the original model.

8: A00009 Fokker-Planck Dynamics in the Energy Domain1, GCINA MAVIMBELA, Dept of Physics and Astronomy, Ohio University, HORACIO E. CASTILLO, Dept of Physics and Asatromony, Ohio University, CLAUDIO CHAMON, Physics Dept, Boston University — We derive a Fokker-Planck Equation (FPE) in the energy domain for a system in an infinite heat bath by coarse-graining its microscopic Master Equation. The resulting FPE carries information on the dynamics through a function $\lambda(E)$, which is a sum over all possible transitions given a state of energy $E$. We investigate the effects of changing the assumptions about the transition rates without changing the Hamiltonian of the model. By determining the eigenvalues of the equivalent Schrodinger Equation (SE), we get the relaxation spectrum of the FPE. We find that in the thermodynamic limit the equivalent SE approaches the classical limit, and we use the WKBJ approximation to solve it. We illustrate the use of the method by applying it to several examples, including a system of harmonic oscillators, and a paramagnet in an external magnetic field.

9: A00010 Doing the Impossible: Very Rare Events in the Harmonic Measure. DAVID ADAMS, LEONARD SANDER, ROBERT ZIFF, University of Michigan — We have developed a method of obtaining accurate data of rare events using biased sampling of random walkers. We have robust the harmonic measure, analogous to the perpendicular electric field on a charged conductor, for percolation, Ising model, and Diffusion Limited Aggregation (DLA) clusters. We measured probabilities down to $10^{-300}$ for percolation and Ising model clusters. These small probabilities allowed us to verify the theoretical predictions for the harmonic measure made by Duplantier. For DLA, which has no theory, we obtained probabilities down to $10^{-110}$. The previous lowest probability was obtained using iterative conformal maps and was limited to small clusters and comparatively high probabilities. For all systems we have obtained the generalized dimension $D_q$, the singularity spectrum $f(\alpha)$, and the distribution of probabilities.
10:00 AM A9.00011 Anisotropic 2-dimensional Robin Hood model. SERGEY BULDYREV, GABRIEL CWILICH, FREDY ZYPMAN, Department of Physics - Yeshiva University — We have considered the Robin Hood model introduced by Zaitsev [1] to discuss flux creep and depinning of interfaces in a two-dimensional system. Although the model has been studied extensively analytically in 1-d [2], its scaling laws have been verified numerically only in that case. Recent work suggest that its properties might be important to understand surface friction [3], where its 2-dimensional properties are important. We show that breaking the rotational symmetry between the different ways of introducing that anisotropy lead to different exponents and scaling laws, in analogy with directed percolation, with which this model is closely related [4]. We show that breaking the rotational symmetry between the x and y axes does not change the scaling properties of the model, but the introduction of a preferential direction of accretion (‘robbing’ in the language of the model) leads to new scaling exponents. [1] S.I.Zaitsev, Physica A189, 411 (1992) [2] M. Paczuksi, S. Maslov and P.Bak, Phys Rev. E53, 414 (1996) [3] S. Buldyrev, J. Ferrante and F. Zypman Phys. Rev E64, 066110 (2006) [4] G. Odor, Rev. Mod. Phys. 76, 663 (2004).

10:12 AM A9.00012 A Cellular Automaton Model of Catastrophic Failure1. C. A. SERINO, W. KLEIN, Boston University — We introduce a two-dimensional cellular automaton model for studying the catastrophic failure of materials under stress. Our model is similar to the Olami-Feder-Christensen earthquake model [Z. Olami et al., Phys. Rev. Lett. 68, 1244 (1992)] except that after a site fails f-times, it no longer can receive stress from its neighbors. In the limit that the interaction range, R, goes to infinity, our model is equivalent to the global load sharing fiber bundle model of Pierce [F. T. Pierce, J. Text. Ind. 17, 355 (1926)] and Daniels [H. E. Daniels, Proc. Roy. Soc. London A 183, 405 (1945)]. By varying the interaction range, we observe two qualitatively different failure modes. For R ≈ 1, catastrophic failure resembles a nucleation-like event which grows symmetrically from a single initiating site and fails every site in the lattice. In contrast, for R ≈ 1 a percolating cluster of failed sites spans the system despite the many active sites that persist, even after catastrophic failure. We use the stress-fluctuation metric to study the ergodicity of our model and hence the validity of equilibrium descriptions of fracture.

1Supported by the department of energy, grant number DE-FG02-95ER4498

10:24 AM A9.00013 Heat transport in quantum spin chains: the relevance of integrability1. JINSHAN WU, MONA BERCU, UCSB — Heat transport in quantum spin chains is investigated through the master equation in Lindblad form derived from the Schrödinger equation of a system coupled with two baths via the projector operator technique. We find that the Fourier’s Law of heat transport is obeyed in some systems. Although a general proof has not been established, after a survey of various quantum spin chains, our results suggest the criteria of anomalous heat transport is not the integrability of the Hamiltonian, but whether or not it can be mapped to non-interacting fermions.

1This work was supported by the Research Corporation, A. P. Sloan Foundation, CHA NanoElectronics, CPI and NSF.

10:36 AM A9.00014 Hard-core Bosons in time-varying traps. ADITYA RAGHAVAN, University of Southern California, MARCOS RIGOL, Georgetown University, STEPHAN HAAS, University of Southern California — We present a study of the time evolution of hard-core bosons (HCBs) in a one-dimensional, time-varying optical trap. Previous results have shown that one-dimensional HCBs can form superfluid and Mott-insulator phases. Using an exact numerical approach, we study the dynamics of the system when the trap curvature is modulated. We find the dynamics to be markedly different in the two phases, and address its relevance in the observation of these phases in optical lattice experiments.

10:48 AM A9.00015 Control of Transport Behavior in spin-1/2 Heisenberg Systems. LEA SANTOS, Yeshiva University — A complete understanding of transport behavior in many-body systems is one of the utmost challenges in fundamental studies of non-equilibrium statistical mechanics. In the classical domain, it is widely believed that chaotic systems should show diffusive transport, whereas integrability should be associated with ballistic transport. In the quantum domain, the conditions that determine specific transport behaviors are still under debate. Here, we analyze transport of local magnetization in finite spin-1/2 Heisenberg systems. By adjusting parameters in the Hamiltonian, these quantum systems may show both integrable and chaotic limits. We provide examples of chaotic systems leading to diffusive and also to ballistic transport. In addition, we develop schemes to control the transport behavior in these systems, showing that quantum control methods may be used to induce a transition from diffusive to ballistic transport.

Monday, March 16, 2009 8:00AM - 11:00AM
Session A10 DMP: Focus Session: Ferroelectrics I

8:00 AM A10.00001 First-principles modeling of closure domains in ferroelectric ultrathin films1. JAVIER JUNQUERA, Universidad de Cantabria — Capacitors based on ferroelectric perovskites are potentially attractive for nanoelectronic devices. However, in many cases their use depends on the stability of a ferroelectric state with an out-of-plane polarization. The interplay between mechanical and electrical boundary conditions, and the local chemistry at the surface or interface might give rise to exotic patterns of the polarization, especially in the thin film regime. The screening of the interfacial polarization charges by real metallic electrodes has been extensively discussed in the literature. We have carried out first-principles computations on two other screening mechanisms in ultrathin capacitors made of a few unit cells of BaTiO3 with metallic SrRuO3 electrodes. First, the simulation of the energetic, structural, and electronic properties of ferroelectric domains in short circuit. The domains are stabilized down to two unit cells, adopting the form of a domain of closure, common in ferromagnetic thin films. The domains are closed by the in-plane relaxation of the atoms in the first SrO layer of the electrode, that behaves more like SrO in highly polarizable SrTiO3 than in metallic SrRuO3. Even if small, these lateral displacements are essential to stabilize the domains, and might provide some hints to explain why some systems break into domains while others remain in a monodomain configuration. An analysis of the electrostatic potential reveals preferential points of pinning for charged defects at the ferroelectric-electrode interface, possibly playing a major role in films fatigue. The closure domain structure, predicted also by other phenomenological and effective Hamiltonian models, is more general than expected. Second, the possibility of screening by a surface state or metallization of the first few layers of the ferroelectric without a top electrode is also explored.

1Work done in collaboration with P. Aguado-Puente, and supported by MEC under Project No. FIS2006-02261
8:36AM A10.00002 Polarization Switching at the Intrinsic Coercive Field of PbTiO$_3$ by Changing Oxygen Partial Pressure 1, M. HIGHLAND, T.T. FISTER, M.-I. RICHARD, D.D. FONG, J.A. EASTMAN, S.K. STREIFFER, P.H. FOUSS, G.B. STEPHENSON, Argonne National Laboratory, Argonne, IL, CAROL THOMPSON, Dept. of Physics, Northern Illinois University, DeKalb, IL — Previously we have found that changing the partial pressure of oxygen in the gas above ultrathin PbTiO$_3$ films on SrRuO$_3$ can induce inversion in the sign of the polarization. Here we present x-ray measurements that allow us to determine the polarization magnitude and domain distribution during switching. For films of thickness above ∼5 nm, switching occurs by the usual mechanism of nucleation and growth of 180° domains having the same polarization magnitude but opposite signs. However, in thinner films switching of the polarization occurs without nucleation; the polarization magnitude decreases to zero and changes sign uniformly without domain formation, indicating that the intrinsic coercive field (E$_{JC}$) is reached. Since E$_{JC}$ has never been reached in oxide ferroelectrics using applied electric field, our results suggest that the barrier to nucleation is large during chemical switching. Work supported by the Dept. of Energy under Contract DE-AC02-06CH11357.

8:48AM A10.00003 Understanding the surface reconstruction during chemical switching of ultrathin PbTiO$_3$ films from density functional theory 1, JUN HE, BRIAN STEPHENSON, SERGE NAHKMANSON, Argonne National Laboratory — First-principles calculations are used to understand the structure and energetics of the newly discovered 4×1 surface reconstruction that forms under reducing conditions during chemical switching of the ferroelectric polarization in ultrathin films of PbTiO$_3$ with SrRuO$_3$ bottom electrodes coherently strained to SrTiO$_3$ (001). Relaxed surface structures are obtained for polar films with various oxygen stoichiometries in the outermost PbO layer. To model the behavior of many-unit-cell thick films, which are observed to have polarizations near the bulk value, the lowest unit cell(s) of the PbTiO$_3$ film are forced to be polar. The observed surface reconstructions are compared with experimental synchrotron x-ray measurements.

9:00AM A10.00004 First-principles calculations of structural energetics of Pb-O divacancies in PbTiO$_3$ and their role in up-down asymmetry of thin films 1, O. PAZ, S. P. BECKMAN, D. VANDERBILT, K. M. RABE, Rutgers University — Defects have been proposed as an important influence on the performance of technologically relevant ferroelectric (FE) materials, even at low concentrations. In PbTiO$_3$, V$_{Pb}V_{O}$ vacancy pairs (VPs) are neutral defects, with a local electric dipole moment that can couple to the bulk polarization. To investigate the role that these defects might play in imprint behavior (i.e., a history-dependent up-down asymmetry), we carried out first-principles supercell calculations of VPs in PbTiO$_3$. While previous works considered a cubic host $\Sigma$ we study the tetragonal FE case for periodic arrays of $\Sigma$ and $\Sigma$-neighbor VPs at densities as low as 3%. Our lowest energy VP is a $\Sigma$-neighbor one oriented so as to break the bulk symmetry between the up and down polarization states. Other VP arrangements are higher in energy by at least 0.2 eV. Atomic relaxation is of particular importance in lowering the energy of the $\Sigma$ below that of the $\Sigma$-neighbor VP. Berry-phase polarization calculations reveal that the total polarization is only slightly modified for VPs whose dipoles are aligned with the polarization, but is significantly suppressed by antialigned VPs.

9:12AM A10.00005 Study on the electro-optic effect in Pb(Zr,Ti)O$_3$ (001) film using spectroscopic ellipsometry 1, TAE DONG KANG, Department of Physics, New Jersey Institute of Technology, XIAO BO, VITALIY AVRUTIN, UMIT OZGUR, HADIS MORKOC, Department of Electrical and Computer Engineering, Virginia Commonwealth University, JUN WOO PARK, HO SUK LEE, HOSUN LEE, Department of Physics, Kyung Hee University, South Korea, XIAOYU WANG, DAVID SMITH, Department of Physics, Arizona State University — Spectroscopic ellipsometry was applied to study electro-optic effect in lead zirconate titanate (PZT) thin films grown epitaxially on Nb-doped SrTiO$_3$ (001) substrates by radio frequency magnetron sputtering. Multilayer model analysis was applied to extract the ordinary and extraordinary refractive indices of the PZT thin film with electric field applied along the (001) direction. The effective linear and quadratic coefficients at a wavelength of 632.8 nm were estimated to be $-134.6 \times 10^{-12}$ m/V and $8.5 \times 10^{-18}$ m$^2$/V$^2$, respectively, while the individual linear electro-optic coefficients $\gamma_{33}$ and $\gamma_{34}$ were -157.1 and 22 pm/V, respectively. We attributed existence of the linear electro-optic effect in unpoled PZT films to the presence of a built-in polarization and simultaneous poling during ellipsometric measurements.

9:24AM A10.00006 A first-principles study of enhancement of polarization with electric field in tetragonal PbTiO$_3$ 1, ANINDYA ROY, Rutgers University, MASSIMILIANO STENGEL, UCSB, DAVID VANDERBILT, Rutgers University — We present first-principles calculations of the electric polarization and $c/a$ ratio of ferroelectric tetragonal PbTiO$_3$ as an external electric field is applied parallel to the polarization direction. The work is motivated in part by experimental observations showing an anomalous enhancement (i.e., nonlinear piezoelectric response) in the $c/a$ ratio for electric fields above $\sim$200 MV/m in PbZr$_{0.2}$Ti$_{0.8}$O$_3$. Working here with pure PbTiO$_3$ for reasons of computational convenience, we calculate the strain response to an electric field applied parallel to the spontaneous polarization. We focus mainly on the case of fixed in-plane lattice constants, which appear most suitable to the experimental conditions, but we also study the case in which all lattice constants are relaxed. In addition explore the effects of artificial negative pressure, with and without the in-plane epitaxial constraint. Two ab-initio computer codes are used for this purpose, and the results are compared to each other and to the experiment.


9:36AM A10.00007 Polarization reversal and backswitching kinetics in epitaxial ferroic thin films 1, JIANHENG LI, BRUCE WESSELS, Northwestern University — Polarization reversal and backswitching kinetics were investigated in epitaxial ferroelectric BaTiO$_3$ thin films. Using the electro-optic effect to monitor domain dynamics, the dynamic response was measured as a function of bias pulse magnitude and temperature. The dynamics followed a Kohlrausch-Williams-Watts (KWW) stretched exponential function in time. From the measurements the activation field for polarization reversal and the activation energy for domain motion were determined. The measured activation energy of 6-12 kJ/mol is in good agreement with prior experiments on bulk material and recent theoretical calculations using molecular dynamics simulations.

Supported by NSF DMR-0605292
Thickness dependent ferroelectric properties of ultrathin BaTiO$_3$ thin films

D.A. FELKER, H.W. JANG, C.B. EOM, M.S. RZCHOWSKI, University of Wisconsin - Madison — The thickness dependence of the coercive field and the spontaneous polarization were studied for epitaxial trilayer heterostructures with SrRuO$_3$ and ultrathin BaTiO$_3$ ferroelectric layers grown on TiO$_2$ terminated (001) SrTiO$_3$ substrates. The BaTiO$_3$ thickness ranged from 2.4 (6 unit cells) to 50 nm. The 3.2 nm (8 unit cells) sample provides the thinnest direct electrical measurement of ferroelectricity in BaTiO$_3$ in a device structure, showing the thickness dependence of ferroelectric properties down into the ultrathin regime and providing a new experimental upper bound on the critical thickness. The coercive field increases dramatically in thinner samples consistent with the Kay-Dunn model of domain nucleation and propagation. Below 10 nm the spontaneous polarization decreases with decreasing thickness due to decreasing screening of the depolarization field by the electrodes. For barriers thicker than 10 nm the polarization decreases due to strain relaxation in the ferroelectric barrier. We discuss these measurements, as well as the temperature dependence of the coercive fields and hysteresis loops.

10:00AM A10.00009 Temperature dependence of the dielectric properties of strained barium strontium titanate films for tunable microwave applications

LISA A. ALLREDGE, WONTAE CHANG, STEVEN KIRCHOEFER, JEFFREY POND, Naval Research Laboratory — Understanding strain effects is critical to achieve desirable dielectric properties in ferroelectric films, which are of interest for tunable microwave applications. Sputter-deposited Ba$_{1-x}$Sr$_x$TiO$_3$ films on (001) MgO were studied in various strain states: in-plane or out-of-plane tetragonal lattice distortions. The optimal system calibration for microwave measurements changes greatly with temperature, requiring frequent recalibration. A temperature-dependent intercalation calibration technique was developed to increase the efficiency of measurements taken as a function of temperature. The films showed significant differences in the ferroelectric phase transition due to lattice distortions, with a strong temperature dependence of the in-plane dielectric behavior for films under tensile strain and a weak temperature dependence for films under compressive strain. We believe that films under tensile strain have polarizations aligned parallel to the applied electric field and so the in-plane dielectric properties are strongly coupled with the field, while films under compressive strain have polarizations perpendicular to the field, resulting in minimal influence on the in-plane dielectric behavior.

10:12AM A10.00010 Density functional study of ferroelectric-electrode interfaceal effects on the stability of ferroelectricity in thin-films

WISSAM A. AL-SAIDI, University of Pennsylvania, ALEXIE KOLPAK, Yale University, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania — Ferroelectric (FE) thin-films are very promising materials for various technological applications. The continuous demand of miniaturization of devices based on FE thin-films by the micro-electronic industry demands an understanding of the critical thickness of ferroelectricity in thin films. Using an ab initio density-functional approach, we study the properties of several capacitor-like structures which are based on Pt/TiO$_2$ and BaTiO$_3$ ferroelectric materials. Different electrodes are used in our study to gain a thorough understanding of the electrode-ferroelectric interfaces, and the role of the interfacial chemical bonding and charge transfer in stabilizing the FE polar phase. We finally used our ab initio results to develop a phenomenological predictive model based on a Landau-Ginzburg-Devonshire functional.

10:24AM A10.00011 Boundary conditions on ferroelectricity in ultrathin SrTiO$_3$ films on silicon

ALEXIE KOLPAK, FRED WALKER, JAMES REINER, CHARLES AHN, SOHRAB ISMAIL-BEI, Yale University, CRISP COLLABORATION — The properties of SrTiO$_3$ films epitaxially grown on Si(001) are strongly influenced by the electronic structure of the interface. Using density functional theory, we demonstrate the presence of an intrinsic interface dipole, the direction of which is independent of the particular combination of Sr, Ti, O, and Si atoms at the interface, and therefore independent of growth conditions. As a result of this intrinsic dipole, a local, positive polarization is induced in the SrTiO$_3$ interfacial region, fixing the electrostatic boundary conditions at the interface and preventing the formation of a negatively polarized state with a single domain. We suggest ways in which this constraint on the ferroelectric behavior can be overcome by interfacial cation doping, allowing for the integration of ferroelectricity with traditional silicon-based devices.

Boundary conditions on ferroelectricity in ultrathin SrTiO$_3$ films on silicon

10:36AM A10.00012 Strain Effect in the Problem of Critical Thickness for Ferroelectric Memory

A.M. BRATKOVSKY, Hewlett-Packard Labs, Palo Alto, A.P. LEVANYUK, U Autonoma Madrid, Spain — We account for inhomogeneous strains while calculating two characteristic thicknesses arising in the problem of critical thickness for ferroelectric memory. One of them marks the stability limit of metastable single domain state under zero external voltage with respect to small fluctuations (spinodal point of the single domain state.) The second one appears when the energies of the single and multidomain state become equal while the latter is considered within one-sinusoidal approximation [1]. At this thickness the single domain state remains metastable, but one may hope that the lifetime of this state becomes suitable for the memory applications[2]. We use the Landau approach for elastically isotropic solid with a single electrostriction constant to illustrate general behavior. It is found that the effect of the elastic strains is qualitatively different for free-standing films versus films on substrates.


10:48AM A10.00013 Unusual polarization patterns in flat epitaxial ferroelectric nanoparticles

IVAN NAUMOV, ALEXANDER BRATKOVSKY, Hewlett-Packard Laboratories — We investigate the effects of a lattice misfit strain on a ground state and polarization patterns in flat perovskite nanoparticles (nanoslands of BaTiO$_3$ and PbZr$_{0.5}$Ti$_{0.5}$O$_3$) with the use of an ab-initio derived effective Hamiltonian. We show that the strain strongly controls the balance between the depolarizing field and the polarization anisotropy in determining the equilibrium polarization patterns. Compressive strain favors 180° stripe/tweed domains while a tensile strain leads to in-plane vortex formation, with the unusual intermediate phase (s) where both ordering motifs coexist [1]. The results may allow to explain contradictions in recent experimental data for ferroelectric nanoparticles. [1] Ivan Naumov and Alexander M. Bratkovsky, Phys. Rev. Lett. 101, 107601 (2008).
8:00AM A11.00001 Coverage-Dependent Faceting of Au Chains on Si(557) , F. J. HIMPEL, J. BARKE, F. ZHENG, S. BOCKENAUER, K. SELL, V. V. OEYNHAUSEN, K.H. MEINES-BRÖER, Dept. of Physics, University of Wisconsin Madison, 1150 University Ave, Madison, WI 53706; Institut fuer Physik, Universitaet Rostock, Germany — The structural and electronic phase diagram of Au on Si(557) is established using scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES). Five phases consisting of altogether seven facets are observed in the sub-monolayer regime. Four of them consist of two coexisting structures. In order of increasing Au coverage the five phases are: Si(111)7×7 + Si(112), Si(557)×2-Au, Si(111)5×2-Au + Si(335)-Au, Si(111)√3×√3-Au + Si(335)-Au, and Si(111)√3×√3-Au + Si(5 5 11)-Au. The relative surface areas of the five phases and seven facets are determined accurately by depositing a Au wedge ranging from 0 to 0.8 monolayer and performing automatic pattern recognition on large-scale STM images. Angle-resolved photoemission spectra are decomposed into contributions from the five phases. The Fermi wave vectors of various facets are identified. Using Si(557)×2-Au as reference we find a coverage of 3 Au chains per unit cell for the frequently-studied Si(111)5×2-Au surface (instead of the widely-used value of 2 Au chains). The impact of this finding on structural models is discussed.

8:12AM A11.00002 The Alignment of Gold Nanorods in Macroscopic Domains , JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, ASHISH AGARWAL, NICHOLAS KOTOV. Chemical Engineering, University of Michigan — The uniform alignment of nanoparticles in domains with macroscopic length scales is critical to the production of self-assembled composite metamaterials for optical applications. We describe methods of self-assembly leading to films and suspensions with a high loading of orientationally ordered nanoparticles in macroscopic domains. The nanoparticles are short aspect ratio gold nanorods, with both plasmon peaks in the visible spectrum. Orientational order can be achieved via applied electric field, mechanical strain, as well as via interactions with anisotropic hosts and among nanoparticles. We have determined the orientational order in our samples from polarized absorbance measurements.

8:24AM A11.00003 Role of the three Si suboxides at the surface of Si quantum dots and in Si/SiO$_2$ quantum wells on optical response of nanoparticles were fabricated with this technique.

8:36AM A11.00004 Formation of Colloidal Nanoparticle Superlattices in a Two Solvent System , CHENQUANG LU, AUSTIN AKEY, IRVING HERMAN, Columbia University — A two solvent system consisting of a high boiling point solvent and a low boiling point solvent was found to greatly aid the self-assembly of nanoparticle superlattices. Nanoparticle mixtures were prepared under multiple suitable solvent evaporation conditions and the products were analyzed by TEM and SEM. The formation process of various binary nanoparticle superlattices was investigated to elucidate the optimal conditions for self-assembly. Superlattice formation in this two solvent system was further investigated with various spatial confinement conditions. Here, the capillary effect during the evaporation of solvents may be the driving factor in the self-assembly. Micrometer scale superlattices of CdSe nanoparticles were fabricated with this technique.

8:48AM A11.00005 Modeling the Self-assembly of Nanorod Superlattices , ALEXEY TITOV, PETR KRAL. University of Illinois at Chicago — Colloidal semiconductor CdSe/CdS nanorods (NR) of diameters of 3-10 nm and lengths of 4-40 nm typically self-assemble into nematic and smectic phases, which are parallel to the substrate, or simple hexagonal (SH) superlattices, which are perpendicular to the substrate [1-2]. We model the formation of these structures by semi-classical means, starting from the forces between the nanorods, their coupling to the substrate and to the external electric fields. We determine the conditions under which superlattices with different number of particles, number of monolayers, aspect ratios of nanorods, etc. can be observed [3], and show that the obtained results agree well with the available experimental data. Our previous results of modeling superlattices of self-assembled monodisperse nanoparticles are also presented.

References:

9:00AM A11.00006 Morphology of Cu$_2$S-CdS and Ag$_2$S-CdS Nanorod Heterostructures , DENIS DEMCHENKO, Virginia Commonwealth University, BRUCE SADTLER, University of California, Berkeley, HAIMEI ZHENG, A. PAUL ALIVISATOS, LIN-WANG WANG, Lawrence Berkeley National Laboratory — A partial cation exchange has been used to synthesize Cu$_2$S-CdS and Ag$_2$S-CdS nanocrystal heterostructures, with two very different morphologies. Cu$^+$ cation exchange takes place preferentially at the ends of CdS nanorods, Cu$_2$S segments grow into the nanorod from both ends. Ag$^+$ exchange is non-selective, Ag$_2$S islands nucleate and grow over the entire surface of the nanorod. This leads to very different patterns, striped Ag$_2$S-CdS superlattice with several equidistant Ag$_2$S segments in a CdS nanorod, and an asymmetric Cu$_2$S-CdS heterostructure with Cu$_2$S segments at the ends of the CdS nanorod. We use first-principles calculations to obtain formation energies of the different epitaxial interfaces between Cu$_2$S-CdS and different facets of CdS nanorods. Comparison of chemical and elastic contributions to the interface formation energy for the Cu$_2$S-CdS heterostructure shows that the relative stability of the interfaces determines the nucleation of Cu$_2$S and the resulting morphology. Furthermore, since two end facets of CdS nanorod are not crystallographically equivalent a controlled asymmetric nucleation of Cu$_2$S can occur.

9:12AM A11.00007 Self-assembly of molecular wires , ANDREAS Riemann, Western Washington University, WESTERN WASHINGTON UNIVERSITY COLLABORATION — Scanning Tunneling Microscopy (STM) has been used to study the self-assembly of the naturally occurring amino acid L-methionine on different surfaces. It has been found that methionine forms highly regular structures on an Ag(111) surface under UHV conditions as well as on a graphite surface under ambient conditions. Methionine arranges itself into an array of molecular wires of uniform width and separation. The spacing of these wires can be controlled by means of the deposition amount. Molecular mechanics calculations are used to suggest a model for the methionine configuration on the surfaces. The width of the wires is determined by two methionine molecules arranged with their carbonyl group facing each other. The regular separation of individual wires suggests a long range interaction between these wires.
9:24AM A11.00008 An STM Study of Atomic Co Wires, NADER ZAKI, DENIS POTAPENKO, Columbia University, PETER JOHNSON, DANDA ACHARYA, PERCY ZAHL, PETER SUTTER, Brookhaven National Lab, RICHARD OSGOOD, Columbia University — Due to stronger electron-electron interactions, 1-D systems are predicted and, in some cases, have been shown to exhibit unique and exotic electronic properties. One route to the formation of 1-D systems is by self-assembly using low-index vicinal crystal surfaces. In this regard, we have successfully formed 1-atom wide Co wires using Cu(775), a 7-atom wide stepped array with (111) terraces. Contrary to a recently reported DFT prediction, the Co wires are not laterally encapsulated but are positioned exactly at the step edge. We will present STM studies of this system performed at room temperature and STS measurements made at low temperature. While vicinal Cu(111) does exhibit “friz” at the steps when scanning above cryogenic temperatures, the Co wires pin the edges, visually accentuating their presence under STM. Furthermore, we observe a lower local density of states for the Co wires as compared with the Cu steps, which also serves to differentiate the two metals. Cu(111) possess a surface projected bandgap which may electronically decouple the wire electrons that reside in this gap. However, we also see resonances at the Fermi level which suggests electronic coupling between the vicinal Cu surface and the Co electrons.

9:36AM A11.00009 III-V nanowires grown in a simple, homebuilt system.1, M. D. SCHROER, J. R. PETTA, Princeton University — Semiconductor nanowires are promising experimental platforms for studying quantum transport due to their built-in, one-dimensional confinement of charge carriers. To enable the study of III-V semiconducting nanowires, we built a simple tube furnace based MOCVD reactor. Growth of InP and InAs nanowires using trimethylindium, di-tert-butylphosphine and triethylarsenic has been studied as a function of temperature, pressure, precursor concentration and growth substrate. At optimal growth conditions, wires of 20-60 nm in diameter and up to 10 μm in length are achievable on InAs substrates. Characterization was performed using SEM, EDS and TEM; both wurtzite and zincblende structures have been observed. We will also present transport measurements of nanowires grown using this system.

1We thank Hongkun Park, Stephen Weinman, and Chun Liang Yu for helpful discussions. This work was supported by the Army Research Office (W911NF-08-1-0189) and the National Science Foundation MRSEC Program through the Princeton Center for Complex Materials

9:48AM A11.00010 Fabrication of nanowire-nanotube hybrid arrays in porous aluminum oxide membranes, ZUXIN YE, HAIHONG CHEN, ISABEL SCHULTZ, WENHAI WU, D. G. NAUGLE, I. LYUKSYUTOV, Texas A & M University — Fabrication of ordered nanowire-nanotube hybrid arrays embedded in porous anodic aluminum oxide (AAO) membranes is demonstrated. Arrays of TiO2 nanotubes were first deposited into the pores of AAO membranes by an electroless sol-gel technique. For subsequent electrochemical deposition of Co nanowires into the TiO2 nanotubes, a thick Au layer was first evaporated on one surface of the membrane to serve as the cathode. Co nanowires were then electrochemically deposited into the TiO2 nanotubes through the other surface to form the hybrid nanowire-nanotube arrays. SEM and TEM measurements showed a high Co nanowire filling factor and a clean interface between the Co nanowires and the TiO2 nanotubes. The TiO2 nanotubes were found to be composed of nanometer sized TiO2 crystals, while the Co nanowires were polycrystalline with Co crystal size comparable to the nanowire diameter. This technique can be extended to the fabrication of hybrid arrays of various materials. This work was supported by DOE No. DE-FG02-07ER46450, NSF No. DMR-0606529, and the Robert A. Welch Foundation A-0514.

10:00AM A11.00011 First Observation of Quantum Size Effects in Metal Films on Insulator, HAWONG HONG, Argonne National Laboratory, AARON GRAY, University of Illinois, Urbana-Champaign, RUQING XU, University of Illinois, Urbana-Champaign, and Hobart and William Smith Colleges — It has long been a goal of the materials science community to study quantum size effects in metal films on insulators and metals. Here the first observation of the quantum effects in metal films on insulators will be reported. Pb thin films, which exhibit the most dramatic quantum-size-effects were chosen again for this effort. Sapphire (001) substrates were used after they were annealed at 1500 °C in air and cleaned in a UHV chamber by heating. X-ray diffraction was measured during and after the deposition-annealing processes. Most of the structural aspects observed with Pb on Si(111) also appeared in Pb films on sapphire. The preferred island heights (or magic heights) appeared as 7, 10, 12, 14 layers from the preliminary analysis. This contrasts the magic heights on the Si substrates (5, 7, 9, . . .). This difference is coming from the phase shifts of confined electrons through the different interfaces. This magic selection of island-heights stays quite strong even at elevated temperatures up to 200–300 °C. Time resolved 3-D reciprocal space mapping also showed very strong ordering between islands during deposition and annealing of the films.

10:12AM A11.00012 Surface Dislocation of Al Films on Ag(111), BO XU, ERKUANG ZHU, CHAO LU, YONGJUN TIAN, Yanshan University — Ordered dislocation structures of metal surfaces are of particularly interests because they can provide templates for building nanostructures with novel electronic, magnetic, and catalytic properties. Here we report two dislocation structures formed for Al on Ag(111). Depending on substrate temperature, Al films demonstrate distinct surface structures. At room temperature, Al nanocrystals with the (111) orientation are formed. At 500 K, a herringbone reconstruction, similar with the well known Au(111) reconstruction surface, is formed, while at 600K, a trigonal reconstruction surface is formed. Molecular self assembly processes on these surfaces are investigated.

10:24AM A11.00013 Theoretical Analysis of Equilibrium Surface Segregation in Ternary III-V and II-VI Semiconductor Nanostructures, SUMEET PANDEY, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We present an atomic-scale analysis of equilibrium surface segregation in ternary compound (III-V and II-VI) semiconductor nanostructures. The analysis is based on a computational scheme for compositional and structural relaxation that combines Monte Carlo with conjugate-gradient methods according to properly modified/extended parameterizations of the valence-force-field (VFF) description; the VFF parameterizations employed in the analysis are validated by comparison with first-principles density functional theory calculations. We report equilibrium concentration distributions in slabs of InxGa1-xAs and ZnxSe1-xS, as a function of composition, x, slab thickness, and slab surface crystallographic orientation, as well as in InxGa1-xAs and ZnxSe1-xS nanocrystals with well-defined surface facets as a function of x and nanocrystal size. The results are discussed in the context of synthesis of core/shell structures of ternary compound semiconductor nanocrystals for increased quantum-dot photoluminescence efficiency.

10:36AM A11.00014 Growth and optical properties of highly oriented ZnSSe alloy nanowires, SUI KONG HARK, YAO LIANG, The Chinese University of Hong Kong — ZnS, ZnSe and their alloys are important semiconductors for optical applications in the UV-blue spectral range. Nanowires, nanobelts and nanotubes of ZnS and ZnSe, but rarely their alloys, had been synthesized, typically as a random, inhomogeneous assembly. For future basic studies and applications, it is necessary to control the orientation and composition of the nanowires. We have grown ZnSSe alloy nanowires epitaxially on GaAs substrates by metal-organic chemical vapor deposition. Their orientation was adjusted by changing the crystallographic orientation of the substrate. Through controlled alloying, they have also achieved band gap engineering. The nanowires were characterized by SEM, HRTEM and XRD. Their optical properties were studied by Raman, cathodoluminescence and photoluminescence spectroscopy. In addition to the nanowires, the growth conditions and optical properties of ZnSSe alloy nano-tetrapods were studied.

2Partially supported by a grant from the Research Grants Council of the Hong Kong Special Administrative Region, China (Project No. 411807)
Controlled Synthesis of Functional Nanostructures, CHRIS PALMSTROM, Uni. of Minnesota — No abstract available.

**8:36AM A12.00002 Kinetic Monte Carlo Simulations of Nanostructure Evolution During Unstable Growth on Patterned GaAs(001)**

CHUAN-FU LIN, KRISTA COSERT, AJMI HAMMOUDA, University of Maryland, HUNG-CHIH KAN, National Chung-Cheng University, Taiwan, ROC, RAY PHANEUF, University of Maryland — We present results of kinetic Monte Carlo simulations, which include a diffusion barrier, lateral atom interaction energy, and Ehrlich-Schwoebel barrier to investigate unstable growth for comparison with our observations on patterned GaAs(001) surfaces at typical growth conditions [1-3]. Our results show a profound change in the mode by which an initial lithographic pattern evolves during growth, with growth mounds dominating at low temperatures and island nucleation and growth at higher temperatures. We describe the use of height-height correlation maps as a tool to facilitate the statistical characterization of the evolution of periodic patterns during growth, and correlate peaks in the maps with the change in growth mode with temperature.


**8:48AM A12.00003 Nanopatterning as a Probe of Unstable Growth on GaAs(001)**

KRISTA COSERT, CHUAN-FU LIN, AJMI HAMMOUDA, University of Maryland, HUNG-CHIH KAN, National Chung-Cheng University, Taiwan, ROC, KANAKARAJU SUBRAMANIAM, CHRIS RICHARDSON, Laboratory for Physical Sciences, RAY PHANEUF, University of Maryland — We report on observations of unstable growth on patterned GaAs(001) surfaces. For growth at 500°C, 1 ML/sec and an As2/Ga beam equivalent pressure ratio of 10:1, we find that grooves oriented at right angles to [110] produce a build up of ridges of GaAs at the upper edges, while for grooves oriented at right angles to [110] no ridges form; instead cusps evolve at the bottoms of such grooves [1]. The cusp-forming grooves show a pronounced initial amplification of depth during growth which changes with height/width ratio and becomes more narrow. The ridge-forming grooves instead broaden during growth. We compare these experimental observations with kinetic Monte Carlo simulations in which a small anisotropic Ehrlich-Schwoebel barrier is included. [1] T. Tadayyon-Eslami, H.-C. Kan, L. C. Calhoun and R. J. Phaneuf, Phys. Rev. Lett. 97, 126101 (2006)

**9:00AM A12.00004 Optimization of air-assisted CVD growth of vertically-aligned ZnO nanowires, guided by structural analysis using X-ray scattering**

JONG G. OK, A. JOHN HART, Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA — ZnO nanowires (ZNWs) are of significant interest for applications ranging from optical sensors to vibrational energy harvesters, due to properties including UV photoluminescence and piezoelectricity. We have studied low-pressure growth of ZNWs using a vapor transport method in air flowing within a tube furnace, giving vertically-aligned ZNW arrays on sapphire substrates seeded by Au catalysts. The growth rate and the average length of ZNWs depend on the flow rate of air and the total growth time, while multiple parameters such as catalyst thickness, pressure, and temperature also interdependently affect the ZNW characteristics. Grazing incidence small-angle X-ray scattering (GI-SAXS) measurements enable non-destructive quantification of ZNW diameter and alignment. By fitting GI-SAXS images using analytical models of the array as a population of solid cylinders having a Gaussian diameter distribution, we establish precise relationships between the structural characteristics and the growth conditions; for example, we determine rates of radial growth and size distribution broadening in comparison to axial growth. Control of the temperature gradient within the furnace also enables growth of well-aligned arrays at substrate temperatures as low as 600°C.

**9:12AM A12.00005 Influence of impurities on phase transition in quasi-one-dimensional nanowires on Si surface**

GEUNSEOP LEE, WOOSANG LEE, HYUNJOO SHIM, Inha University, Korea, SANG-YONG YU, JA-YONG KOO, Korea Research Institute of Standards and Science, Korea — We investigated using low-energy electron diffraction the influence of impurity doping on the structural phase transition in an array of quasi-one dimensional In nanowires on Si(111). A clean Si(111)×1 surface, in its pristine form, undergoes a structural phase transition into a 8×2 phase below 120 K. Introducing various impurities (hydrogen, oxygen, and alkali metals) on the surface at room temperature was found to affect the 4×1-to-8×2 structural phase transition by changing the transition temperature (Tc). Adsorption of the two types of the gases affected the transition in opposite ways: hydrogen adsorption lowered the Tc, whereas oxygen adsorption raised the Tc. Dosing of different alkali metals (Na, K, and Li) all decreased the Tc. Usually, impurities are expected to suppress the phase transition into the symmetry-broken phase (the low-temperature phase) by acting as random fluctuations in structure. In this sense, the increase in Tc by the oxygen adsorption is an exceptional case enhancing the phase transition. Possible mechanisms leading to different influences of the various impurities on the structural phase transition of this In/Si(111) will be discussed.

**9:24AM A12.00006 Numerical simulations of VLS heteroepitaxial nanowire growth**

VIVEK SHENOY, Brown University. KLAUS SCHWARZ, JERRY TERSOFF, IBM T. J. Watson Center — Nanowires are particularly attractive for designing heterostructures, as effective radial strain relaxation allows heterostructures with a wider range of material combinations. The electrical, optical, and thermal properties of the nanowire are highly dependent on the accurate control of the locations and thicknesses of such heterostructures. However, in the case of nanowire growth from a metal seed particle, the composition of the seed particle will vary for growth of different materials due to alloying, which may cause problems in controlling interface abruptness. Also, recent experiments have shown that in many cases, growth instabilities do not allow for the formation of nanowires with desired morphology and material combinations. We have developed a continuum model for the growth of heteroepitaxial nanowires, and we use it to study the factors that control interface abruptness and instabilities during growth. Our model includes the following features that are critical for capturing the composition profiles in nanowires: 1) the differences of the attachment rates of the alloy components at the catalyst-wire interface, 2) the possibility of miscibility gap in the alloy phases of the catalyst and the nanowire, 3) composition dependence of the surface energies of the nanowire and nanowire-catalyst interface and 4) anisotropy in surface energies leading to faceted morphologies.
9:36AM A12.00007 Three Dimensional, Single-crystal, Oxide NANOFENCES for Epitaxial Growth of Electronic, Magnetic or Electromagnetic Nanoscale-Devices¹. AMIT GOYAL, SUNG-HUN WEE, KARREN MORE, ELIOT SPECHT, ORNL — A unique, three-dimensional (3D), single-crystal, MgO, NANOFENCE comprised of single crystal MgO nanowire units was synthesized via epitaxial growth on (100) SrTiO₃ substrates. Individual single crystal MgO nanowire units comprising the nanofence were observed to have high aspect ratios with small diameters of 10-20 nm and long lengths from 100 nm up 1 μm. X-ray diffraction shows that the 3D MgO nanofence has an epitaxial relation with (100) SrTiO₃ substrates with only a single {100} <100> orientation and with full-width-half-maximum values of (200) ω-scan and (110) φ-scan with 4.5° and 5.5°, respectively. Such nanofences offer a single crystal, 3D nanotemplate for epitaxial growth of wide-ranging, 3D, electronic, magnetic and electromagnetic nanodevices.

¹Research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory (ORNL), managed by UT-Battelle, LLC for the U. S. Department of Energy.

9:48AM A12.00008 Hierarchical Assembly of Epitaxial Quantum Dot Nanostructures on Templated Substrates. ROBERT HULL, Rensselaer Polytechnic Institute — Using the focused ion beam (FIB), we have modified the local topography and chemistry of Si(100) surfaces, and demonstrated control of the geometry, size, location and proximity of epitaxial Ge(Si) quantum dot (QD) nanostructures which are nucleated on these templated surfaces. We show how QDs can be located with a precision ~ 10 nm using local Ga⁺ FIB doses ~ 10¹⁵ cm⁻², and how QD size and morphology can be modified by local surface chemistry. We further describe how growth kinetics can control formation of more complex nanostructures with internal length scales bridging the ∼ 10 nm dimensions necessary for application to potential nanoelectronic device architectures and dimensions that are accessible through external lithography. In particular, we describe the self assembly of “quantum dot molecule” (QDM) GeₓSi₁₋ₓ nanostructures where a four-fold QD structure forms around shallow strain relieving pits. Positional control of these QDMs using external lithographic templating allows formation of hierarchically assembled systems with length scales ranging from ∼ 10 nm in QD size and proximity, through the ∼ 100 nm dimensions of the QDM, to the micro/macro-scopic dimensions accessible with external lithography. We also describe methods for electronic and magnetic functionalization of these nanostructures by separation of ion species from alloy liquid metal sources in a mass selecting FIB column. This allows generation of ion beams comprising electronically non-invasive species for nanoscale surface templating (e.g. Si, Ge), electronic doping (e.g. As, B), or spin doping (e.g. Mn). Application of such structures to potential novel nanoelectronic device structures will be discussed. This work is done in collaboration with J. Floro, J. Graham, M. Gherasimova, J. Thorp (UVA), F. Ross (IBM), A. Portavoce (CNRSS), M. Kammier (U. Duisburg) and J. Gray (U. Pittsburgh).

10:24AM A12.00009 Fabrication Methods for Positioning of Quantum Dots¹. REBECCA KRAMER², RUPERT OULTON, VOLKER SORGER, NITIPAT PHOLCHAI, University of California, Berkeley, XIANG ZHANG, NSF Nanoscale Science and Engineering Center, University of California, Berkeley — Quantum dot positioning is highly useful in terms of integrating nanoelectromitters into nanostructures, such as nanocavities and quantum dot waveguides. Demonstration of control over the positioning of quantum dots has proven difficult, and consequently construction of single-photon emitting systems has been hindered. We report the ability to reliably position nanoscale functional objects, specifically quantum dots, within a well-defined location. Programmed assembly of DNA linked quantum dots on both gold and silver substrates is obtained by Electron Beam Lithography patterning and a series of surface chemical functionalizations. A single quantum dot was successfully positioned within 100 nm of the desired location in 36 percent of the experiments. Furthermore, the method was completely reproducible within 500 nm accuracy. This method has the potential to functionalize quantum dots in even smaller pattern sizes.

¹Support for this work was provided by NSF NSEC (DMI-0327077)
²This work was done at Berkeley, however the author is now affiliated with Harvard University.

10:36AM A12.00010 Stress-driven self-assembly of Si-based nanomembranes for on-chip applications. FRANCESA CAVALLO, Leibniz-Institut für Festkörper- und Werkstofforschung Dresden, Helmholtzstrasse 20, 01067-Dresden, Germany, RUDEESAN SONGMUANG, YONGFENG MEI, ARMANDO RASTELLI, OLIVER SCHMIDT, Leibniz-Institut für Festkörper- und Werkstofforschung Dresden, Helmholtzstrasse 20, 01067-Dresden, Germany — A new field of Si technology based on transferable and engineered nanomembranes has developed with the realization of the fact that properties of bulk Si are preserved in nm-thin layers released from the substrate surface. We demonstrate the ability to pattern Si-based films with nano-scale features, and fold them into a predetermined 3D configuration by finely tuning the strain distribution in the membranes by well-established deposition processes, i.e., MBE, PVD, and thermal oxidation. Our major contributions are the fabrication of integrated microtube resistors based on Si:B/SiGe:B tubes; the use of the Ge condensation technique to tailor the strain distribution in SiGe films on insulator; the manufacturing of fully scalable and CMOS compatible—self—seeding hybrid tubes; the fabrication of linear and circular networks formed by interconnected wrinkled structures; the experimental demonstration of light emission from Ge and Si nanoparticles integrated in a tube wall; the observation and investigation of the waveguiding effect along the axis of SiOx/Si tubes.

10:48AM A12.00011 Isotropic and anisotropic strain-induced self-assembled oxide nanostructures. MARTA GIBERT, PATRICIA ABELLAN, ALESSANDRO BENEDETTI, FELIP SANDIUMENGE, TERESA PUIG, XAVIER OBRADORS, Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, 08193 Bellaterra, Catalunya, Spain — The apparition of new functionalities based on size- and shape-dependent properties requires strategies for the formation of well-defined structures at nanometric scale. We have developed a bottom-up low-cost chemically-derived methodology based on the control of strain and surface energies anisotropies in CeO2/LAO system to tune the lateral aspect ratio, orientation and kinetics of interfacial oxide nanostructures. Self-organized uniform square-based nanopyramids form under isotropic strain [1]. In contrast, highly elongated nanostructures (long/short axis ∼ 20) grow induced by biaxial anisotropic strain and anisotropic surface energies. Island’s distinct crystallographic orientation is the clue of their differentiated shape, and also influences their distinct evolution. The kinetically-limited coarsening of isotropic nanodots contrasts with the ultrafast kinetics of anisotropic islands. Experimental analyses are based on AFM, TEM, XRD and RHEED, and simulations based on a thermodynamic model enable us to confirm the equilibrium shape of each sort of island’s shape in relation to its misfit strain and surface characteristics. [1] Gilbert, M. et al., Adv.Materials 19 (22), 3937 (2007).

Monday, March 16, 2009 8:00AM - 11:00AM –
Session A13 DCOMP: Focus Session: Metropolis Thesis Prize and Multiscale Modeling

8:00AM A13.00001 Flexibility and Direction Reversal in Flapping Locomotion. SAVERIO SPAGNOLIE, UC San Diego, MICHAEL SHELLEY, New York University — In order to better understand the role of flexibility in the flapping of wings and fins in Nature, experimentalists at NYU have studied a heaving foil with passive pitching. We analyze this system numerically, having constructed a high-order accurate numerical scheme to solve the full Navier-Stokes equations in two-dimensions to study the dynamics. We are able to reproduce qualitatively the results of the experiments: by increasing the flapping frequency, we find regions of improved performance when compared to a rigid wing, regions of under-performance, and a bi-stable regime where the flapping regime can move horizontally in either direction. The numerical simulations have led to predictions of other modes of flapping locomotion, which have subsequently been observed in experiments. We also find that a symmetry breaking transition to forward flapping flight, as observed in experiments of a heaving foil with no pitching, may be directed with only very slight flexibility.
8:12AM A13.00002 Modeling the combined effect of surface roughness and shear rate on slip flow of simple fluids , ANOOSHEH NIARVARANI, NIKOLAI PRIEZEJ, Michigan State University — Molecular dynamics (MD) and continuum simulations are carried out to investigate the combined effect of shear rate and surface roughness on interfacial slip in simple fluids. For weak wall-fluid interaction energy, the nonlinear shear rate dependence of the slip length in a flow past atomically flat surfaces is obtained from MD simulations. Both the magnitude of the slip length and the slope of its rate-dependence are significantly reduced in the presence of periodic surface roughness. Continuum simulations are used to reproduce the behavior of the effective slip length in a flow over periodically corrugated surface at low shear rates. The continuum analysis includes the functional form of the slip length vs. local shear rate computed from MD simulations. The discrepancy between MD and continuum results at higher shear rates is explained by examination of local velocity profiles and pressure distribution along the wavy surface.

8:24AM A13.00003 KMC simulations in 3+1 dimensions and the effects of attachment probabilities and potential gradients on island morphologies , CHRISTOPHER FLECK, JUDITH YANG, University of Pittsburgh, ALAN MCGAUGHEY, Carnegie Mellon University, JUN REN, University of Pittsburgh — Thin film growth and nano-oxidation have received significant attention lately, especially given the interesting nature of Cu$_2$O growth. Our long-term vision is for a comprehensive, fundamental understanding of a gas-surface reaction via coordinated multi-scale theoretical and in situ experimental efforts. The link between the theoretical and experimental efforts is our kinetic Monte Carlo (kMC) code that simulates general behavior of the irreversible nucleation and growth of epitaxial islands. This simulation was originally a versatile 2+1 dimensional KMC code (Thin Film Oxidation or TFOx) that considered a wide range of elementary steps, including deposition, adsorption, dissociation of gas molecules, surface diffusion, aggregation, desorption, and substrate-mediated indirect interactions between static adatoms. Recently, TFOx has been extended to a 3+1 dimensional KMC code composed of a C++ console program and Python GUI, such that parameterized testing, parallel execution, and 3D growth capabilities are feasible. Emphasis has been placed on the effects of the potential gradient, multilayer nucleation and sticking parameter on the 3D island morphology.

8:36AM A13.00004 Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics Talk: Understanding Nano-scale Electronic Systems via Large-scale Computation , CHAO CAO, University of Florida — Nano-scale physical phenomena and processes, especially those in electronics, have drawn great attention in the past decade. Experiments have shown that electronic and transport properties of functionalized carbon nanotubes are sensitive to adsorption of gas molecules such as H$_2$, NO$_2$, and NH$_3$. Similar measurements have also been performed to study adsorption of proteins on other semiconductor nano-wires. These experiments suggest that nano-scale systems can be useful for making future chemical and biological sensors. Aiming to understand the physical mechanisms underlying and governing property changes at nano-scale, we start off by investigating, via first-principles method, the electronic structure of Pd-CNT before and after hydrogen adsorption, and continue with coherent electronic transport using non-equilibrium Greens function techniques combined with density functional theory. Once our results are fully analyzed they can be used to interpret and understand experimental data, with a few difficult issues to be addressed. Finally, we discuss a newly developed multi-scale computing architecture, OPAL, that coordinates simultaneous execution of multiple codes. Inspired by the capabilities of this computing framework, we present a scenario of future modeling and simulation of multi-scale, multi-physical processes.

9:12AM A13.00005 Role of Adatom Relaxations in Computing Lattice-gas Energies: Multisite Interactions , RAJESH SATHIYANARAYANAN, T. L. EINSTEIN, Univ. Maryland, College Park — In simple lattice-gas models, only nearest-neighbor pair interactions are used to model adatom interactions. However, multisite interactions, such as trios and quartos, are necessary to understand certain surface properties like the orientation dependence of step stiffness and the equilibrium shape of islands. Strong multisite interactions are found to be present on a variety of metallic surfaces. Unlike pair interactions, the relaxations of adatoms in a multisite interaction are not along bond directions. Hence, these adatoms can shift significantly from their high-symmetry positions, making multisite interactions more sensitive to relaxations. Using VASP calculations, we showed that trios are very sensitive to lateral adatom relaxations on Pt(111) and Cu(100). Our recent calculations on Cu(110) indicate that in addition to trios, quartos also undergo a big change due to adatom relaxations. Such findings severely limit the effectiveness of lattice-gas models in characterizing surface interactions. We discuss alternate approaches to this problem.

9:24AM A13.00006 Rapid and Accurate Estimates of Alloy Phase Diagrams for Design and Assessment , TECK TAN, DUANE JOHNSON, University of Illinois, Urbana-Champaign — Based on first-principles cluster expansion (CE), we obtain rapid but accurate estimates of alloy T vs c phase diagrams from a mean-field theory that conserves sum rules over pair correlations. Such conserving mean-field theories are less complicated than the popular cluster variation method, and better reproduce the Monte Carlo (MC) phase boundaries and T$_c$ for the nearest-neighbor Ising model [1]. The free-energy f(T,c) is a simple analytic expression and its value at fixed T or c is obtained by solving a set of n non-linear coupled equations, where n is determined by the number of sublattices in the groundstate structure and the range of pair correlations included. While MC is “exact,” conserving mean-field theories are 10 to 100$^3$ faster, allowing for rapid phase diagram construction, dramatically saving computation time. We have generalized the method to account for multibody interactions to enable phase diagram calculations via first-principles CE, and its accuracy is showed vis-a-vis exact MC for several alloy systems. The method is included in our Thermodynamic ToolKit (TTK), available for general use in 2009. [1] V. I. Tokar, Comput. Mater. Sci. 8 (1997), p.8

9:36AM A13.00007 Chemistry effects on dislocation mobility in refractory bcc metals , NICHOLAS KIOUSSIS, ZHENGZHENG CHEN, Department of Physics, California State University, Northridge, GANG LU, Department Mechanical and Aerospace Engineering, University of California Los Angeles — Using a novel concurrent multiscale approach we demonstrate that the local environment of transition-metal solutes in refractory bcc metals has a large effect on the mobility and slip paths of dislocation. The results reveal that solid solutes or nano-clusters of different geometries may lead to solid-solution hardening (SSH) or softening (SSS), in agreement with experiment, including spontaneous dislocation glide and activation of new slip planes. The underlying electronic mechanism is also studied by the multiscale approach. Solutes nano-cluster can affect Peierls potential surface (PPS) dramatically. The results indicate that it is the change of the anisotropy of the lattice resistance induced by solutes that result in the different behavior of the dislocation according to the different geometries of solutes nano-clusters.
9:48AM A13.00008 Computational studies of thermal evolutions of extended interstitial defects in silicon.¹
HYOUNGKI PARK, JOHN W. WILKINS, The Ohio State University — Annealing induces the nucleation of extended defect clusters in silicon and their evolution, where clusters grow by capturing or interchanging interstitials, and change their crystallographic structure in order to minimize the formation energy. Extensive molecular dynamics (MD) simulations and first-principle nudged elastic band (NEB) simulations explore the thermal transitions from one structure to another of three energetically competing extended interstitial defects: two rod-like defects \{311\} and \{111\}, and Frank dislocation loop. MD simulations capture critical sequences of atomic processes during transitions from \{311\} and \{111\} defects to Frank loops as their atomic configurations and habit planes change, and massively parallelized NEB simulations within the local density approximation reveal the energetics of reaction barriers.

¹Supported by DOE-Basic Energy Science. Computing resources are provided by NERSC and OSC.

10:00AM A13.00009 Multiscale Modeling of Catalysis and its Application to Hydrogen Production through the Water Gas Shift Reaction on Nanoparticles¹
ALTAF KARIM, JAMES T. MUCKERMAN, Brookhaven National Lab — We describe a density functional kinetic Monte Carlo approach enabling us to study and simulate the steady-state condition of the water gas shift (WGS) reaction on Cu and Au nano-particles supported on ZnO(0001) surfaces. We have adopted a multiscale modeling paradigm in which density functional theory can be used to determine the behavior of systems at much larger length and time scales by coupling it with kinetic Monte Carlo methods. In the first step, density functional theory is used to obtain the energetics of the relevant atomistic processes of the WGS reaction on Cu and Au nanoparticles. Subsequently, the kinetic Monte Carlo method is employed, which accounts for the spatial distribution, fluctuations, and evolution of chemical species under steady-state conditions. Our simulations show that, in agreement with experiments, the hydrogen production rate strongly depends on size and structure of the nanoparticles.

¹DOE, Division of Chemical Science, Contract No. DE-AC02-98CH10886 and NERSC computational resources

10:12AM A13.00010 Preparation of nanoporous systems for the study of the mechanical properties of silica aerogels by Molecular Dynamics simulations
JOHN S. RIVAS MURILLO, Department of Mechanical and Aerospace Engineering, West Virginia University, MARTINA E. BACHELECHNER, Computer Science, Math and Physics Department, Fairmont State University, EVER J. BARBERO, Department of Mechanical and Aerospace Engineering, West Virginia University — This presentation focuses on the application of the Molecular Dynamics technique to study the mechanical properties of silica aerogels through the simulation of a tension test. It covers multiple areas, including aspects related to the preparation of a well-relaxed nanoporous system from the expansion of an amorphous bulk sample and the influence of the initial configuration of the system on the final results of the simulated tension test. The results presented here will help to develop a more complete procedure to prepare a proper sample for the study of the mechanical properties of a nanoporous system by using Molecular Dynamics. Comparison of the simulation results and previously published experimental data is provided.

10:24AM A13.00011 A hierarchical DPD thermostat to avoid over and/or underdamping at long wavelengths in MD simulations
KEVIN GREEN, COLIN DENNISTON, MARTIN MUSER, University of Western Ontario — In this talk, we present a new approach to use dissipative particle dynamics as a thermostat in molecular dynamics simulations. The main idea is to have DPD act on groups of atoms so that damping can be tuned as a function of length scale. This allows one to achieve a quality factor of vibrations, which is barely wavelength dependent. The number of floating point operations per time step is orders of magnitude less for the new approach than for regular DPD or any other thermostat acting on individual particles. In addition, the method avoids both underdamping of natural and/or DPD dynamics at long wavelengths L and overdamping which is unavoidable at large L for Langevin or Nose-Hoover based thermostats. Thus correlation times for observables that live on long wavelengths L, are of order L or rather of order L² as for conventional thermostats.

10:36AM A13.00012 Determination of the ground state structures of binary alloys via global space group optimization (GSGO) with no restrictions on composition: Al-Sc,¹ YOSHIHIDE YOSHIMOTO, Institute for Solid State Physics, University of Tokyo, Japan — Here, we extend the GSGO evolutionary algorithm scheme to survey crystal structures of binary A-B systems without constraint on the AₓBₓ composition. At each generation of the randomly started evolutionary sequences, the formation energy convex hull for the actual population is determined. The search proceeds by replacing the structures farthest away from the convex hull with new ones produced via mating and mutation with no constraints on composition. As a test of this new procedure, we searched the ground state compounds of the Al-Sc alloy whose lattice types are not easily inferred from that of the Al and Sc constituents, respectively fcc and hcp solids. Repeated, independent evolutionary sequences with six and eight atoms in the supercell were performed yielding as ground states respectively B₁₂, and D₀₁₉, B₂, and L₁₀, as known from experiment and previous ab-initio studies. This yields a synthesis of the final convex hull.

¹Work at Northwestern supported by AFOSR. Work at NREL funded by DOE-SC-BES-MSED through NREL Contract DE-AC36-08GO28308

10:48AM A13.00013 Non-crystalline state of silicon studied by multicanonical simulation combined with first-principles calculation
YOSHIHIDE YOSHIMOTO, Institute for Solid State Physics, University of Tokyo, Japan — By combining multicanonical ensemble molecular dynamics and first-principles calculations, non-crystalline state of silicon is studied. This attempt contrast with quenching molecular dynamics simulations whose speed is usually by far quicker than that of experimental quenchings. To make the molecular dynamics simulation tractable, a model interatomic potential is used. The parameter, however, is determined by first-principles calculation so that the discrepancy between the first-principles interatomic potential and the model one is minimized on the typical configuration set of the multicanonical ensemble. Because multicanonical ensemble represents the whole thermodynamics of the system, the obtained model will conserve the thermodynamics to a maximum extent. (thermodynamic downfolding of an interatomic potential [1]) The transition between amorphous silicon and liquid silicon, and the density maximum of liquid silicon as a function of temperature will be discussed. (Silicon has similar structure to that of water) [1] Y. Yoshimoto, J. Chem. Phys., 125, 184103 (2006)

Monday, March 16, 2009 8:00AM - 10:48AM – Session A14 DFD: Instabilities, Turbulence and Nonlinear Flows 315
8:00AM A14.00001 Search for the “ultimate state” in turbulent Rayleigh-Bénard convection for Rayleigh numbers up to $4 \times 10^{13}$ and Prandtl numbers near 0.8$^1$. GUENTER AHLLERS, UCSB, DENIS FUNFSCHILLING, CNRS Nancy, EBERHARD BODENSCHATZ, MPI for Dyn. and Self-org., Goettingen — Measurements of the Nusslet number $N_u$ over the Rayleigh-number range $10^{10} < \text{Ro} < 4 \times 10^{12}$ for $N_2$ (Prandtl number $Pr = 0.72$) and $S_f$ ($Pr = 0.78$ to 0.82) are reported. They were made at pressures up to 15 bars and near-ambient temperatures for a cylindrical sample of height $L = 2.2$ m and diameter $D = 1.1$ m in a new High-Pressure Convection Facility (HPCF) constructed at the Max Planck Institute for Dynamics and Self-Organization in Göttingen, Germany. The data can be represented well by a power law with an effective exponent of 0.31. They do not show the transition to an “ultimate regime” reported by Chavanne et al.

$^1$Work at UCSB supported by NSF Grant DMR07-02111.

8:12AM A14.00002 Large-scale circulation and Nusselt number in turbulent rotating Rayleigh-Bénard convection.$^1$, JIN-QIANG ZHONG, UCSB, RICHARD STEVENS, U. Twente, HERMAN CLERCX, Eindhoven U. Tech., DETLEF LOHSE, U. Twente, GUENTER AHLLERS, UCSB — We present measurements of the large-scale circulation (LSC) and the Nusselt number $N_u$ of turbulent Rayleigh-Bénard convection in a cylindrical cell of aspect ratio 1 and rotated about a vertical axis at a rate $\Omega$. The side-wall temperatures at eight equally spaced azimuthal positions in the horizontal mid-plane were fit to a cosine function that gave the azimuthal LSC orientation $\theta (t)$ ($t$ is the time), the temperature amplitude $\delta (t)$, and the rms amplitude $\delta T (t)$ of the fluctuations about the fits. The LSC precessed in an azimuthal direction opposite to that of the imposed rotation. The precession rate $\omega = d\theta / dt$ showed a sharp transition at a Rossby number $\text{Ro}^*> 2.5$. As $\text{Ro}$ increased, $\delta (t)$, $\delta T (t)$ increased beginning at $\text{Ro}^*$. At $\text{Ro}^*$ $N_u$ began to increase with increasing $\Omega$. At high $\text{Ro} |\omega|$ was proportional to but much smaller than $\Omega$.

$^1$Work at UCSB supported by NSF Grant DMR07-02111.

8:24AM A14.00003 Geometry of turbulence: a stroll through 61,506 dimensions$^1$, PREDRAV CVITANOVIC, JOHN F. GIBSON, Georgia Tech, JONATHAN HALCROW, Inst. for Physical Sciences, McLean, VA 22101 — We propose to use a hierarchy of exact unstable invariant solutions of the Navier-Stokes equations — corresponding to the recurrent coherent structures observed in experiments — to construct a description of the spatio-temporally chaotic dynamics of turbulent fluid flows as a walk through the space of such structures. This description should allow us to obtain quantitative predictions of transport properties of fluid flows such as bulk flow rate and mean wall drag.

$^1$Partly supported by NSF grant DMS-0807574

8:36AM A14.00004 Lagrangian and Eulerian Turbulence: intermittency and Universality, LUCA BIFERALE, University of Rome, ICTR COLLABORATION — We present the result of a high resolution numerical simulations of homogeneous and isotropic turbulence at BIFERALE, University of Rome, ICTR COLLABORATION. The side-wall temperatures at eight equally spaced aircraft were made at pressures up to 15 bars and near-ambient temperatures for a cylindrical sample of height $L = 2.2$ m and diameter $D = 1.1$ m in a new High-Pressure Convection Facility (HPCF) constructed at the Max Planck Institute for Dynamics and Self-Organization in Göttingen, Germany. The data can be represented well by a power law with an effective exponent of 0.31. They do not show the transition to an “ultimate regime” reported by Chavanne et al.

8:48AM A14.00005 Large-eddy simulation of swirling reacting flows, MARCEL ILIE, University of California San Diego — Turbulent, swirling flows are encountered frequently in various chemical engineering processes. In combustion processes swirling flames are of interest due to the fact that provide enhanced mixing and reduce the pollutants formation. The challenge in understanding turbulent swirling flows stems mainly from the complexity of the flow field which is subject to vortex breakdown, recirculation and flow instability. In general the flow instabilities arise at high swirl numbers and can be used to control the performance of combustors. In the present study a large-eddy simulation (LES) approach with Smagorinsky eddy viscosity subgrid scale model is used to predict the swirling flame. The conserved scalar mixture fraction-based thermo-chemical variables are described using the steady laminar flamelet model. The present study shows that LES together with a laminar flamelet model provides a good prediction of the structure of turbulent swirling flames. Also LES captured very well the complex flame structures involving vortex breakdown which leads to swirl-induced recirculation zones, flow instability, and the occurrence of localized extinction. Also, the present study shows that the formation of an elongated recirculation (bluff-body stabilized) zone is strongly dependent on the swirl number and the ratio of momentum in the swirling annulus and central fuel jet.

9:00AM A14.00006 Methods to Approach Velocity Data Reduction and Their Effects on Conformation Statistics in Viscoelastic Turbulent Channel Flows, GAURAB SAMANTA, ANTONY BERIS, University of Delaware, ROBERT HANDLER, Naval Research Laboratory, KOSTAS HOUSIADAS, Aegae University, Greece — Karhunen-Loeve (KL) analysis of DNS data of viscoelastic turbulent channel flows helps us to reveal more information on the time-dependent dynamics of viscoelastic modification of turbulence [Samanta et al., J. Turbulence (in press), 2008]. A selected set of KL modes can be used for a data reduction modeling of these flows. However, it is pertinent that verification be done against established DNS results. For this purpose, we did comparisons of velocity and conformations statistics and probability density functions (PDFs) of relevant quantities obtained from DNS and reconstructed fields using selected KL modes and time-dependent coefficients. While the velocity statistics show good agreement between results from DNS and KL reconstructions even with just hundreds of KL modes, tens of thousands of KL modes are required to adequately capture the trace of polymer conformation resulting from DNS. New modifications to KL method have therefore been attempted to understand the role of the rapid magnetic pressure in the evolution of the Reynolds stresses for different mean distortions and magnetic fields.

9:12AM A14.00007 Study of Influence of Rapid Pressure in MHD Turbulence, SAIKISHAN SURYANARAYAN, AARTHI SEKARAN, Texas A&M University — Turbulence, under the influence of magnetic field is characterized by anisotropy. Relatively limited work has been done in understanding and modeling magnetohydrodynamic (MHD) turbulence. The rapid distortion theory (RDT), which has been employed to study hydrodynamic turbulence, is a limiting case where the gradients of the mean velocity are very high compared to the gradients of the fluctuating field. When analyzed in a spectral framework, this leads to the independent evolution of each Fourier mode. RDT has been used to understand production and more importantly the “rapid” part of the pressure strain redistribution, as the other terms in the Reynolds stress evolution equation become negligible in the rapid distortion limit. Earlier work attempts to characterize the effect of the rapid pressure based on the geometry of the symmetric part of the mean velocity gradient tensor. This work deals with the application of RDT to MHD turbulence. The application of Elsasser variables reorganizes the MHD equations in a form similar to conventional Navier-Stokes. The current work is a numerical study of the Elsasser variable evolution equation in the rapid distortion limit and attempts to understand the role of the rapid magnetic pressure in the evolution of the Reynolds stresses for different mean distortions and magnetic fields.
9:24AM A14.00008 Anisotropic Particles in Fluid Flow1, MONICA KISHORE, Haverford College, NICHOLAS T. OUELLETTE, Yale University, JERRY GOLLUB, Haverford College — Anisotropic particles are common in natural flows. In previous work [1] the dynamics of neutrally buoyant finite-sized spherical particles with Stokes numbers up to 0.08 were examined in 2D flows with Reynolds numbers of 72-220. Here, we extend this work to neutrally buoyant, high-aspect-ratio anisotropic particles of mm to cm length in a 2D cellular flow. The particle trajectories and orientations are tracked simultaneously with the underlying velocity field, which is measured using much smaller tracer particles. These methods allow us to compare the relative velocity and orientation of anisotropic particles to various features of the flow field. We find, for example, that the long axes of the particles preferentially align with the instantaneous direction of maximum compression, and that this alignment increases with particle aspect ratio. [1] N.T. Ouellette, P.J.J. O'Malley, and J.P. Gollub, Phys. Rev. Lett. 174504 (2008).

1Supported by NSF-DMR 0803153.

9:36AM A14.00009 Statistics of preferential particle concentration in free-surface2, JASON LARKIN, WALTER GOLDBURG, University of Pittsburgh, MAHESH BANDI, Center for Nonlinear Studies and Condensed Matter & Thermal Physics Group, Los Alamos National Laboratory — Particles floating on a turbulent surface of water cluster into temporally complex patterns. We experimentally study the statistics of this preferential particle concentration for various Reynolds numbers, for both transient and steady-state dynamics. The probability density function for particle concentration exhibits a power-law with an exponential cut-off. We will discuss our preliminary analysis as to how this distribution depends upon the Reynolds number and the spatial-scale r at which the system is coarse-grained.

2This work supported by National Science Foundation grant DMR NSF 0604477. MMB carried out this work under the auspices of the National Nuclear Security Administration of U.S. Department of Energy at LANL under contract No. DE-AC52-06NA25396.

9:48AM A14.00010 Vortex Street behind an Oscillating Wire on a Soap Film, AARON MEYER, ILDOO KIM, X.L. WU, University of Pittsburgh — A von Kármán vortex street, a periodic array of vortices behind a bluff body is normally characterized by a single frequency $f_0$ at which the vortices shed. In this study, von Kármán vortex streets are generated on a 2D soap film using a glass-covered metal wire in a static magnetic field. When the wire is driven with electric current to make an oscillatory motion with frequency $f$, transverse to the mean flow, vortices shed at a frequency $f'$ differs from $f_0$. It is seen that with oscillation, $f_0$ is suppressed, $f'/f_0$ becomes a rational number, and vortices are rearranged to form an exotic spatial structure. This “frequency-locking” phenomena show some features of the sine-circle map, but the relevancy to the physical system is not clear. When the amplitude of the oscillation is large enough, the system becomes chaotic. In this chaotic regime, the energy power spectrum resembles that of 2D decaying turbulence.

10:00AM A14.00011 An Anomalous Behavior in Vortex Shedding in a Flowing Soap Film, ILDOO KIM, X.L. WU, University of Pittsburgh — It is generally believed that von Kármán vortex street is characterized only by Reynolds number $Re = UD/v$, where $U$ is the mean flow speed, $D$ is the size of the body which generates the vortex street, and $v$ is the kinematic viscosity. In this study, we present experimental data in a flowing soap film showing that changing $U$ with fixed $D$ and changing $D$ with fixed $U$ are not equivalent to each other, suggesting that $Re$ alone is not sufficient to characterize vortex shedding by a bluff body. The velocity of eyes of the vortices relative to the mean flow, normalized by $U$, increases when we increase $D$, but decreases when we increase $U$. It is also found that the longitudinal spacing between the eyes is a linear function of $D$, but independent of $U$.

10:12AM A14.00012 Rayleigh-Taylor Instability in Nonlinear Optics, SHU JIA, JASON W. FLEISCHER, Princeton University — We demonstrate, theoretically and experimentally, an all-optical Rayleigh-Taylor instability. By applying a polar (Madelung) transformation to the nonlinear Schrödinger equation for paraxial beams, we identify fluid density with light intensity and fluid velocity with the gradient of the optical phase. Pressure is obtained by using a self-defocusing nonlinearity in a photorefractive crystal, while acceleration is created by imposing a refractive index gradient. In this way, we are able to control the effective gravity, pressure, and input density ratio. The perturbed interface at the output is then studied as functions of these parameters. Observations of the characteristic spatial period show excellent agreement with analytical calculations from perturbation theory. In this case, wave diffraction, rather than viscosity or surface tension, sets the scale for long-wave growth. Further, we show that compressibility effects are important and demonstrate that care must be taken regarding shock-wave formation. The results hold for any Schrödinger fluid, e.g. superfluids and quantum plasma, and lay the foundation for a variety of fluid-inspired instabilities in nonlinear optics.

10:24AM A14.00013 Dispersive shock waves with negative pressure, WENJIE WAN, DMITRI DYLOV, CHRISTOPHER BARSI, JASON FLEISCHER, Princeton University — Dispersive shock waves (DSWs) arise from nonlinear wave breaking and mode dispersion and are a fundamental type of fluid behavior. In normal fluid systems, the pressure is positive and repulsive, so that the underlying particles resist compression. Examples include water, plasma, and optical beams with self-defocusing nonlinearity. However, there are systems in which the interactions are attractive, resulting in an effectively negative pressure. Here, we demonstrate that dispersive shock waves can arise in these negative-pressure systems by considering the equivalent optical problem with self-focusing nonlinearity. Using partially-coherent light, to prevent the competition of modulation instability, we experimentally observe DSWs formed in a self-compressive beam in a photorefractive crystal. We characterize the nonlinear speed and profile of the DSWs, and show that statistical de-phasing by the incoherent beam causes an effective Landau damping of the waves. Observations are supported both by analytic theory and numerical simulation.

10:36AM A14.00014 Convective instability in pipe flow through a sudden expansion, JAMES SEDDON, University of Manchester — Flow through a sudden expansion in a pipe has been the subject of a lot of recent scientific interest. The geometry occurs in many industrial processes, from heat exchangers to combustion chambers, and is closely related to the physiological problem of flow through a stenosis. The inlet flow from the upstream pipe is Poiseuille, which forms a central jet surrounded by a recirculating eddy in the expanded downstream pipe. Recently we showed that this kind of flow passes through a symmetry breaking bifurcation before the onset of both intermittent and fully periodic time-dependent effects. We have now investigated the intermittency in more detail and find that the flow becomes convectively unstable. A wave packet emerges from the laminar state and grows to a maximum size of several diameters before decaying.

Monday, March 16, 2009 8:00AM - 11:00AM – Session A15 DFD: Soft Matter, Fluid Structure and Properties 316
8:00AM A15.00001 Impact of a viscous drop, WENDY W. ZHANG, ROBERT D. SCHROLL, University of Chicago, CHRISTOPHE JOSSENDRO, STEPHANE ZALESKI, UMR 7190, Institut d'Alembert — Recent experiments [1] reveal that reducing the ambient air pressure entirely suppresses the splash generated by the impact of an oil drop at several m/s onto a dry smooth wall. Motivated by these observations, we simulate two types of drop impact: impact onto a smooth, dry solid wall and head-on collision of two identical liquid drops. In both cases we make the additional simplification that impact simply arrests the downward fall and redirects the liquid radially outwards in a thin, expanding sheet. It does not break the drop surface. Since experiments suggest that splash is created by airflow deforming the thin sheet, we focus on the time-evolution of the thin liquid sheet but restrict ourselves to one simpler situation of negligible airflow effects. In this regime, we find that the ejected sheet is always characterized by two different length-scales. Surface tension controls the rim size. The thickness over the rest of the sheet is controlled by a different mechanism. Impact onto a solid surface creates a pancake whose thickness is controlled by viscous dissipation. Head-on collision creates a sheet that thins continuously with distance from the collision center. Its thickness is controlled by the kinematics of impact.


8:12AM A15.00002 Focused impact through layers of aqueous cornstarch solution, BIN LIU, Courant Institute, NYU, JUN ZHANG, Dept. of Physics and Courant Institute, NYU, MICHAEL SHELLEY, Courant Institute, NYU — A layer of aqueous cornstarch solution, when punched with a solid sphere, will create a thickened mass on the sphere that transmits the impact towards the bottom. As a consequence, the mass can leave an imprint on the bottom, if composed of a soft molding clay. The impact transmitted through the fluid layer is more localized for slower speeds of the sphere, giving rise to an imprint with sharper curvature. Our work shows that a layer of shear-thickening fluid may help to focus the impact rather than dissipate it when punched slowly enough.

8:24AM A15.00003 Drop pinch-off of concentrated surfactant solutions in the lamellar phase, ITAI COHEN, Cornell University, PATRICK SPICER, MARCO CAGGIONI, P&G, JOHN SAVAGE, Cornell University — Droplet pinch-off in air is a common phenomenon that occurs all around us. At the point of pinch-off, the drop radius shrinks to zero in a finite amount of time. The pressure exerted by the interface is inviscid, and thus finite, and the fluid velocity is zero at the drop radius. Although the fluid velocity becomes singular at Pinch-off in Newtonian fluids, this finite time singularity gives rise to universal features in the pinch-off process that can be described by similarity solutions for the fluid flow. In this talk I will address the question of how this process is altered when observed in concentrated surfactant solutions that are in the lamellar phase. Remarkably we find that pinch-off in these systems is a mix between universal and non-universal behavior.

8:36AM A15.00004 Watching the Paint Dry: Dynamics of Drying in Porous Media, LEI XU, Harvard University, SIMON DAVIES, ICI, ANDREW SCHOFIELD, the University of Edinburgh, DAVID WEITZ, Harvard University — What is the dynamics of drying in porous media? It has been difficult to visualize due to the non-transparency of the media. We study this phenomenon in an optical index matched colloidal system with confocal microscopy. We observe abrupt air invasions which result from the strong flow from menisci in large pores to menisci in small pores. The size and structure of the air invasions are in accord with 3D invasion percolation. By varying the particle size and contact angle we unambiguously demonstrate that capillary pressure dominates the drying process.

8:48AM A15.00005 Monitoring Three-dimensional Fluid Configurations in Porous Media, AMBER KRUMMEL, DAVID WEITZ, Harvard University, SCHLUMBERGER COLLABORATION — The spatial and time resolution of confocal microscopy allows us to observe the three-dimensional fluid configurations in the pore. We monitor the time evolution of the fluid configuration with a confocal scope with precise flow and pressure measurements, such that we can begin to understand the origins and consequences of the three-dimensional fluid configurations that evolve in the sample. The porous media used in this work is composed of slightly sintered, borosilicate glass beads that are 150 microns in diameter.

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9:00AM A15.00006 Shear banding fluids in microchannels: high shear rheology, slippage and Poiseuille flow instability, PHILIPPE NGHE, GUILLAUME DEGREG, PATRICK TABLING, MMN, UMR CNRS-ESPCI 7083 Gulliver, ARMAND AIDARI, PCT, UMR CNRS-ESPCI 7083 Gulliver — We characterize by Particle Image Velocimetry the Poiseuille flow a semi-dilute solution of wormlike micelles (a CTAB and sodium nitrate aqueous solution) in pressure resistant microchannels. At low shear rates, we observe a parabolic profile. Increasing the pressure driving the flow, the fluid separates into two phases above a critical shear rate at the wall. This is the so called shear-banding regime. Deducing the non-linear rheology from the velocity profiles by a local calculation, we are able to measure the stress versus shear rate curve at least one order of magnitude above the dynamical range attainable in Couette geometries, independently from the slippage, revealing a strongly shear-thinning structure. In addition, by extrapolation of the velocity profiles to the wall position, we measure an absence of slippage at the wall. Looking into more details to the increase in velocity fluctuations in the downstream direction, we characterize a supercritical instability in this shear-bandied Poiseuille flow, localized at the interface between the two phases with a wavelength comparable to the confining dimension.

9:12AM A15.00007 Nonlinear Dynamics in Viscoelastic Jets, TRUSHANT MAJMUDAR, MATTHIEU VARAGNAT, GARETH MCKINLEY, Massachusetts Institute of Technology — Instabilities in free surface continuous jets of non-Newtonian fluids, although relevant for many industrial processes, remain poorly understood in terms of fundamental fluid dynamics. Inviscid, and viscous Newtonian jets have been studied in considerable detail, both theoretically and experimentally. Instability in viscous jets leads to regular periodic or random aerofoil of the jet, which exhibits a non-trivial frequency dependence with the height of the fall. Here we present a systematic study of the effect of viscoelasticity on the dynamics of continuous jets of worm-like micellar surfactant solutions of varying viscosities and elasticities. We observe complex nonlinear spatio-temporal dynamics of the jet, and uncover a transition from periodic to quasi-periodic to a multi-frequency, broad-spectrum dynamics. Beyond this regime, the jet dynamics smoothly crosses over to exhibit the “leaping shampoo” or the Kaye effect. We examine different dynamical regimes in terms of scaling variables, which depend on the geometry (dimensionless height), kinematics (dimensionless flow rate), and the fluid properties (elasto-gravity number) and present a regime map of the dynamics of the jet in terms of these dimensionless variables.

9:24AM A15.00008 Relating shear banding and orientational order in wormlike micellar solutions, MATTHEW HELGESON, MATTHEW REICHERT, University of Delaware, ERIC KALER, Stony Brook University, NORMAN WAGNER, University of Delaware — Shear banding has been observed in a variety of complex fluids, including polymer solutions, colloidal suspensions and, most prominently, wormlike micelles (WLMs). However, accurate modeling of shear banding fluids remains a challenge, due to the inability to identify the mechanism(s) leading to banding. Using a novel approach that combines measurements of phase behavior, rheology, and spatially-resolved microstructure on model WLMs, we present the first complete study of local rheology and microstructure through the shear banding transition for model WLMs in the vicinity of an equilibrium isotropic-nematic transition (I-N). The rheology of such fluids is well-described by the Giesekus constitutive equation with incorporated stress diffusion, which allows simultaneous description of rheology, flow kinematics, and spatially-resolved microstructure under shear. The results show that shear banding coincides with a first-order, shear-induced transition to a paranematic state at critical values of micellar orientation and alignment, which can be related directly to a non-monotonic constitutive relation. Furthermore, the model allows for the construction of non-equilibrium state diagrams that elucidate a number of experimental observations in shear banding fluids.
9:36AM A15.00009 Structure and Phase Behavior of Ion–Dipole Mixtures. WONKI ROH, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — It is well established that Coulombic interactions induce a liquid–liquid transition in ionic solutions. By contrast, the occurrence of phase separation driven by anisotropic dipolar interactions is still a matter of debate, with our recent simulation results excluding this phase separation for a large region of the temperature–density plane. These observations naturally lead to the question whether phase separation takes place in mixtures that contain ions as well as dipolar particles. Employing large-scale grand-canonical Monte Carlo simulations, we investigate four prototypical ion–dipole mixtures: ion-dominated systems in which the dipole moment is either strong or weak, and dipole-dominated systems with strong or weak dipolar strength. We focus on the low-temperature regime and search for phase separation by varying the chemical potentials of the ions as well as the dipolar particles. Depending on temperature and on the magnitude of the dipole moment, remarkable liquid structures are found that may have implications not only for the behavior of ion–dipole mixtures, but also for self-assembly in suspensions containing charged and dipolar colloids.

9:48AM A15.00010 Surface Layering Near Room Temperature in a Nonmetallic Liquid1, SUDESHNA CHATTOPADHYAY, BENJAMIN STRIPE, PHILIP FRY, GEUNNADI EVMENENKO, PULAK DUTTA, Dept. of Physics & Astronomy, Northwestern Univ., STEVEN EHRlich, HAIDING MO, Brookhaven National Laboratory — Oscillatory density profiles (layers) have been observed at the free surface of nonmetallic liquid metals and alkali metals at and above room temperature [1]. A surface-layered state has been previously reported only in one dielectric liquid, tetrakis[2-(ethylhexyloxy)]silane (TEHOS), and only at lower temperatures [2]. We have used x-ray reflectivity to study a molecular liquid, pentaphenyl trimethyl trisiloxane. Below Tc = 267K (well above the freezing point for this liquid), density oscillations appear at the surface. This liquid has a higher Tc (~1200K) than TEHOS (~950K), so that layers appear at T/Tc = 0.2 in both cases. Our results indicate that surface order is a universal phenomenon in both metallic and dielectric liquids, and that the underlying physics is likely to be the same since layers always appear at T < 0.2Tc, as theoretically predicted [3].

REFERENCES:

1Supported by NSF grant no. DMR-0705137.
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10:00AM A15.00011 Structural effect of sugars on water1, SIMCHA SREBNIK, RAVIT MATZA, ILIYA KUSNER, YOO D. LIVNEY, Technion - Israel Institute of Technology — The modulation of the structure of liquid water by solutes has tremendous consequences in numerous fields, particularly on the stability of proteins. However, the reasons for the differences in effects of similar solutes are still unclear. Recently, Livney and coworkers [1] found a strong relationship between the hydration layer of sugars and its effect on the phase transition of a model polymer, which may be explained by the strong interaction between water and sugars leading either to cooperative structuring of the water and thus to large hydration numbers, or disrupting water structure near the sugar, resulting in lower hydration. Using atomistic Monte Carlo simulation, we studied the compatibility of various sugars with an ideal tetrahedral water structure, as embodied in square ice. Our simulations suggest the following order of compatibility with ideal water structure: galactose > glucose > mannosse. In agreement, experimental measurements of isentropic compressibility show the same order of hydration numbers and kosmotropic effect. A simple physical model of the binary system is used to shed further insight on the structuring effect of sugars on water. 1. Shipgelman, A.; Portnaya, I.; Ramon, O.; Livney, Y. D. J Polym Sci Part B: Polym Phys 2006, 44, 2307-2318.

1Israel Science Foundation is acknowledged for partial support.

10:12AM A15.00012 Reconstructing the dynamical solvent structure around a model ‘hydrated electron’ using inelastic x-ray scattering, R. CORIDAN, G.H. LAI, N. SCHMIDT, Dept. of Physics, P. ABBAMONTE, Dept of Physics, Seitz Materials Research Lab, G.C.L. WONG, Depts. of Mat. Science Eng. and Physics, and Seitz Materials Research Lab, U of Illinois, Urbana-Champaign, R. CODEWAT, S. GARDE, Dept of Chem and Bio Engineering, Rensselaer Polytechnic Institute, M. KRISCH, European Synchrotron Radiation Facility, A.Q.R. BARON, SPRing-8/RIKEN and SPRing-8/JASRI — The structure and dynamics of water on femtosecond timescales is relevant to many topics in physical chemistry such as electron solvation. We computationally reconstruct the A-scale spatial and fs-scale temporal evolution of density fluctuations in water using high-resolution inelastic x-ray scattering (IXS). The imaginary part of density propagator ω is directly extracted from the IXS data, and the real part recovered using Kramers-Kronig relations. The resultant complex-valued χ(q,ω) is the Fourier transform of the real-space density-density response function χ(t) which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We use this density propagator and linear-response theory to reconstruct a model of the hydrated electron. The water density fluctuations as the electron ‘diffuses’ through bulk water can be observed. Moreover, preliminary data on the solvent response to changes in the electronic wave function will be presented.

10:24AM A15.00013 Direct measurement of negative square gradient coefficients for density fluctuations in all-atoms simulations of common liquids, COLIN DENNISTON, LINGTI KONG, DAN VRIESINGA, University of Western Ontario — We perform all-atom simulations of common liquids such as water (TIP3P) and organic liquids such as short-chain olefins. We show that square gradient coefficients for the mass density can be measured directly in a linear response measurement to sinusoidal forces at several different wavelengths. Surprisingly, in all fluids measured, the square gradient coefficient is negative implying that density gradients lower the free energy of the system. However, stability is maintained at any wavelength greater than the separation between molecules due to the global mass conservation constraint. We suggest that this provides a mechanism for the molecular scale cut-off of pressure singularities that arise in situations such as droplet pinch-off.

10:36AM A15.00014 Chiral Structures of Thermoresponsive Soft Spheres in Hollow Cylinders1, MATTHEW A. LOHR, University of Pennsylvania, AHMED ALSAYED, CNRS/University of Pennsylvania, ZEXIN ZHANG, ARJUN G. YODH, University of Pennsylvania — We experimentally observe the formation of closely packed crystalline structures in hollow cylinders. The structures have varying degrees of chiral order. The systems are created from aqueous suspensions of thermoresponsive N-isopropylacrylamide (NIPA) microgel particles packed in micron-scale cylinders. The temperature-tunable diameter of these particles, the system’s volume fraction is changed, permitting observations of the resilience of these structures and their melting transitions. Melting of these thermal crystalline structures is observed. [1] R. O. Erickson, Science 181 (1973) 705-716.

1This work is supported by MRSEC grant DMR-0520020 and NSF grant DMR-080488.

10:48AM A15.00015 Nonlinear Transverse Wave Excitations in Fluid Flows, DILLON SCOFIELD, Dept. Physics, Oklahoma State Univ.; PABLO HUQ, Univ. Delaware — The interplay of inertia and dissipation in flows with nonlinear transverse wave excitations is described by including a vortex field into the stress-energy balance equation. The theory uses an acoustic spacetime which allows limiting the speed of propagation of fluid transverse waves to a maximum speed. In the low speed limit, the theory reduces to the Navier-Stokes equations. By examining other limiting cases we show that the Navier-Stokes theory neglects terms involved with the transport of vorticity and the dissipation of energy due to the vortex field. Comparison of the theory to experiment, relative to the Navier-Stokes theory, shows that the presence of the vortex field accounts for the observed relative increase in energy dissipation, extended lifetime of vortex structures, and excitation structure of the transverse wave field.
A simple and systematic characterization of the radio frequency (RF) spectra of homogeneous, paired atomic Fermi gases at general temperatures, experiments on atomic Fermi gases remove ambiguity plaguing the interpretation of previous RF studies. Our calculated spectral intensities are in semi-quantitative agreement with the data.

Fermi gases. Here we establish the underlying physics of these RF measurements. We show that, by providing a clear dispersion signature of pairing, they distinguish between a normal Fermi liquid and a paired superfluid at highly imbalanced gas, and (c) the normal Fermi liquid state for a repulsive, balanced gas. We address the question of how rf spectroscopy can make a sharp distinction between a normal Fermi liquid and a paired superfluid at $T = 0$. We also describe the role of final state interactions and of finite temperature effects.

Supported by NSF DMR-0706203 and ARO W911NF-08-1-0338.

8:24AM A16.00003 Pseudogap phenomena in the BCS-BEC crossover regime of atomic Fermi gases , SHUJNI TUSCHIYA, Department of Physics, Keio University, 3-14-1 Hiyoshi, Yokohama, Japan and CREST(JST), 4-1-8 Honcho, Saitama, Japan, RYOTA WATANABE, Department of Physics, Keio University, 3-14-1 Hiyoshi, Yokohama, Japan, YOJI OHASHI, Department of Physics, Keio University, 3-14-1 Hiyoshi, Yokohama, Japan and CREST(JST), 4-1-8 Honcho, Saitama, Japan — We study pseudogap behavior of atomic Fermi gases in the BCS-BEC crossover. Including pairing fluctuations, we calculate the fermionic density of states above the superfluid transition temperature $T_c$, based on the strong coupling theory developed by Nozières and Schmitt-Rink. We show that the gap structure appears in the density of states above $T_c$ in the crossover region, and it evolves as the attractive interaction strength increases. We also clarify the temperature dependence of the pseudogap, which disappears as the temperature rises, and determine the pseudogap region in the phase diagram. We discuss the origin of the pseudogap by examining the behaviors of quantities such as spectral function and self-energy.

Supported by ARO grant W911NF-08-1-0338.

8:36AM A16.00004 Universal properties of ultracold Fermi gases , SHIZHONG ZHANG, UIUC, ANTHONY LEGGETT — We present some general considerations on the properties of a two-component ultra-cold Fermi gas along the BEC-BCS crossover. It is shown that the interaction energy and the free energy can be written in terms of a single dimensionless function $h(\xi, \tau)$, where $\xi = -(k_F a_s)^{-1}$ and $\tau = T/T_F$. The function $h(\xi, \tau)$ incorporates all the many-body physics and naturally occurs in other physical quantities as well. In particular, we show that the average rf-spectroscopy shift $\delta(\xi, \tau)$ and the molecular fraction $f_c(\xi, \tau)$ in the closed channel can be expressed in terms of $h(\xi, \tau)$ and thus have identical temperature dependence. The conclusions should have testable consequences in future experiments.

Supported by NSF PHY-0555325 and NSF-MRSEC Grant No. DMR-0213745.

9:00AM A16.00006 Temperature and final state effects in radio frequency spectroscopy experiments on atomic Fermi gases , YAN HE, CHIH-CHUN CHIEN, QUINCHEN, KATHY LEVIN, University of Chicago — We present a simple and systematic characterization of the radio frequency (RF) spectra of homogeneous, paired atomic Fermi gases at general temperatures, $T$, in the presence of final state interactions. The spectra, consisting of possible bound states and positive as well as negative detuning ($\nu$) continua, satisfy exactly the zeroth- and first-moment sum rules at all $T$. We show how to best extract the pairing gap and how to detect the $\nu < 0$ continuum arising from thermally excited quasiparticles, not yet seen experimentally. We explain semi-quantitatively recent RF experiments on “bound-bound” transitions, predicting effects of varying temperature.

9:12AM A16.00007 The Higgs resonance in fermionic condensates , ROMAN BARANKOV, Boston University — The Higgs mode appears in the spectrum of fermionic condensates described by the BCS model as a result of the energy dispersion of interaction. Specifically, the mode enters the spectral gap of quasi-particle excitations when the pairing of fermions is enhanced at the Fermi energy. Conversely, it becomes a resonance in the quasi-particle continuum with a finite lifetime, when the pairing is suppressed on the energy scale small compared to the equilibrium gap. The exponential decay of the mode converts into algebraic decay for a smooth suppression. We confirm our analytical results by numerical analysis of the pairing dynamics.

Supported by AFOSR.

SHIQUAN SU, DANIEL E. SHEEHY, JUANA MORENO, MARK JARRELL — We study Feshbach-resonantly interacting fermions near unitarity within the context of the attractive Hubbard model. Our principal focus is the single-particle spectral function for such strongly-interacting fermions, recently probed in radio-frequency spectroscopy and photoemission experiments in cold-atom systems. To obtain quantitatively-accurate results on unitary gases, we apply the Dynamical Cluster Approach (DCA) and the Maximum Entropy method to study this system both in the pair-formation temperature region and in the low-temperature condensed state. Different Quantum Monte Carlo approaches emphasizing different observables are used as the quantum solver in the DCA approach, and the data from different approaches are compared to each other.


9:36AM A16.00009 Feshbach–Einstein condensates

VALY ROUSSEAU, PETER DENTENEER, Instituut-Lorentz, University of Leiden (The Netherlands) — We investigate the phase diagram of a two-species Bose-Hubbard model describing atoms and molecules on a lattice, interacting via a Feshbach resonance. We identify a region where the system exhibits an exotic super-mott phase and regions with phases characterized by atomic and/or molecular condensates. Our approach is based on a recently developed exact quantum Monte Carlo algorithm, the Stochastic Green Function (SGF) algorithm with tunable directionality. We confirm some of the results predicted by mean-field studies, but we also find disagreement with these studies. In particular, we find a phase with an atomic but no molecular condensate, which is missing in all mean-field phase diagrams.

This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

9:48AM A16.00010 Strongly-correlated fermionic matter in the dilute limit

BOGDAN MIHAILA, Los Alamos National Laboratory, ANDRES CARDENAS, Cal Poly Pomona — We study “the ground-state properties of the many-body system composed of spin-1/2 fermions interacting via a zero-range, infinite scattering length contact interaction.” The above is referred to sometimes as the George Bertsch problem, and it is of particular interest in astrophysics in connection with the equation of state for neutron matter and has been revisited recently with the advent of experimental studies of the BCS to BEC crossover in ultracold fermionic atom gases. We will show that new insights into the solution to this problem are obtained in the context of a coupled-cluster (exp S) expansion approach to calculating the equation of state for dilute fermionic systems and that present state-of-the-art Monte Carlo calculations have not yet provided the definitive answer.

10:00AM A16.00011 Superfluid equation of state of state of dilute composite bosons or how to include 3 and 4-body problems in the many-body problem

XAVIER LEYRONAS, ROLAND COMBESCOT — We show how the 3 and 4-body problems emerge in the BEC limit of the BEC-BCS crossover, where we treat explicitly dimers as made of two fermions. We give the argument leading, at zero temperature, to the calculation of the equation of state. We find that, when expanding the chemical potential in powers of the density $n$ up to the Lee-Huang-Yang order, proportional to $n^{3/2}$, the result is identical to the one of elementary bosons in terms of the dimer-dimer scattering length $a_{M}$, the composite nature of the dimers appearing only in the next order term proportional to $n^2$.

10:12AM A16.00012 A study of momentum entanglement and negativity in Bardeen-Cooper-Schrieffer states at finite temperature

CHUN KIT CHUNG, CHI KWONG LAW, Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, Hong Kong SAR, China — We study the momentum entanglement between the spin-up and spin-down particles of the homogeneous Bardeen-Cooper-Schrieffer (BCS) state at finite temperature. To achieve this, we construct from the BCS state the partial transposition $\rho^{T_A}_{\downarrow}$ of the two particle density matrix in momentum space. The structure of $\rho^{T_A}_{\downarrow}$ and its corresponding negativity $N_2$ are examined. We show that $\rho^{T_A}_{\downarrow}$ consists of infinitely many decoupled $2 \times 2$ submatrices, and momentum entanglement coexists with the pairing order parameter $\Delta$. It is found that pairs with momenta slightly above a surface related to the Fermi energy contribute this entanglement most significantly. We propose an entanglement witness operator as a measurable quantity to detect momentum entanglement in BCS states.

10:24AM A16.00013 Matterwave Probe for Detecting Fermi Superfluidity

SATYAN BHONGALE, HAN PU, University of Hong Kong — We propose a matter wave probe for detecting BCS type superfluidity within a trapped two-component Fermi gas. While, previous theoretical/experimental attempts have addressed Fermi superfluidity via a global measurement, for example by demonstrating a vortex lattice, our proposal allows for a local measurement of the pairing gap. For this, we study the phase diagram of a mixture of Bose-Einstein condensate and an interacting two-component Fermi gas. We identify regions of the parameter space where the Bose-Fermi mixture is unstable resulting in phase separation. We show that, under proper conditions, by employing a tunable scattering resonance, the phase separation phenomenon can be exploited as a robust probe of “local” fermion superfluidity.

1 Funded by the W. M. Keck Program in Quantum Materials, Rice University.

10:36AM A16.00014 Detecting Onset of BCS-Superfluidity Using a BEC Probe

B. RAMACHANDRAN, S.G. BHONGALE, H. PU, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, TX 77005, USA — Recent experiments have used Feshbach resonance to tune the interactions in a two-component ultracold Fermi gas to obtain (Bardeen-Cooper-Schrieffer) BCS-type pairing and hence superfluidity. For this degenerate gas, we propose using Bose-Einstein Condensates (BEC) as a matter wave probe of the BCS superfluid state. Towards this end, we explore the phase diagram of a 3-dimensional mixture of BEC and a two-component superfluid fermi gas at finite temperature. In particular, we identify the regime in which the homogeneous mixture becomes unstable against phase separation. We show that, under proper conditions, this spatial phase separation phenomenon occurring in the presence of the BEC can be used to probe the “local” value of the superfluid Gap parameter and possibly help detect the onset temperature of the BCS superfluidity.


10:48AM A16.00015 ABSTRACT WITHDRAWN —
8:00AM A17.00001 Excited-State Spectroscopy and Control of Single Spins in Diamond1, G.D. FUCHS2, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA — Nitrogen Vacancy (NV) defect centers in diamond are a promising system for spin-based applications in quantum information and communication at room temperature. Using a combination of optical microscopy and spin resonance, the spin of individual NV centers can be initialized, manipulated and read out. These techniques have been used to study the long room temperature spin coherence times of NV centers as well as their interactions with nearby electrical and nuclear spins. There remain significant challenges, however, both in understanding the physics of these defects as well as the development of technologies based on their quantum properties. In particular, knowledge of the detailed structure of the orbital excited state, which continues to be an active research area, is critical to ultra-fast quantum control schemes. Here we present recent experiments using single-spin resonant spectroscopy of the excited-state of an NV center at room temperature1 We observe these spin levels over a broad range of magnetic fields allowing for a direct measurement of the zero-field splitting, g-factor and transverse anisotropy splitting. The latter of these is nearly zero in the ground-state spin levels, but plays an important role in the excited-state. In addition, we find strong hyperfine coupling between the nitrogen nuclear spin and the NV electronic spin in the excited-state. These findings will be discussed in the context of quantum control of single and coupled spins in diamond.

1Funding by AFOSR and ARO is gratefully acknowledged.

8:36AM A17.00002 Time-resolved measurements of single electron spins using continuous wave lasers1, PATRICK IRVIN, YANJUN MA, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, JESSE BEREOVSKY, DAVID D. AWSCHALOM, Department of Physics, UC Santa Barbara, Santa Barbara, CA 93106 — Applications such as spin-based quantum computing require that the dynamics of single spins are monitored. Single spins produce a small signal and measurement is further complicated by the background from the large number of neighboring spins. We have developed a time-resolved Kerr rotation technique that uses continuous wave lasers. This technique is able to resonantly address a particular spin. Furthermore, it provides an efficient means of data collection that allows for more signal averaging. Finally, we decrease the background and increase the light-matter interaction by utilizing a solid-immersion lens. We will describe our recent efforts to measure single spins in GaAs/AlGaAs fluctuation-type quantum dots.

1This work was supported by the National Science Foundation.

8:48AM A17.00003 A photonic cluster state machine gun, TERRY RUDOLPH, Imperial College London, NETANEL LINDNER, Technion Institute, SOPHIA ECONOMOU, Naval Research Lab — A method is developed to convert certain single photon sources into devices capable of emitting large strings of photonic cluster state in a controlled and pulsed “on demand” manner. Such sources greatly alleviate the resources required to achieve linear optical quantum computation. Standard spin errors, such as dephasing, are shown to affect only 1 or 2 of the emitted photons at a time. This allows for the use of standard fault tolerance techniques. Using realistic parameters for current quantum dot sources, we conclude high entangled-photon emission rates are achievable, with Pauli-error rates less than 0.2%. For quantum dot sources the method has the added advantage of circumventing the problematic issue of obtaining identical photons from independent, non-identical quantum dots. By using recently controlled-phase gates between two spins in neighboring quantum dots, a two-dimensional cluster can be generated.

9:00AM A17.00004 Complete quantum control of a single quantum dot spin using ultrafast optical pulses, DAVID PRESS, Stanford University, THADDEUS LADD, Stanford University, National Institute of Informatics, BINGYANG ZHANG, Stanford University, YOSHIIHSA YAMAMOTO, Stanford University, National Institute of Informatics — We demonstrate a complete set of ultrafast all-optical single-qubit operations on a single electron spin in a quantum dot [Nature 456, 218 (2008)]. First, the spin is initialized by optical pumping into a pure spin-state with 92% fidelity. Next, a single-qubit gate is implemented by rotating the spin about any arbitrary axis using a sequence of two ultrafast optical pulses separated by a time delay. Finally, the spin is measured by detecting single-photon photoluminescence. As a manifestation of controlling the spin with optical pulses, we demonstrate six complete Rabi oscillations between the two spin states, and a complete set of Ramsey interference fringes. The fidelity of our π/2- and π-rotations exceed 90%. The single-qubit gate is completed in 38 ps, potentially allowing for approximately 10⁸ operations within the qubit’s expected microsecond coherence time, and quantum information processing with clock speeds exceeding 10 GHz.

9:12AM A17.00005 All-optical coherent control and spin-echo of electron spins bound to neutral donors in GaAs, SUSAN CLARK, Stanford University, KAI-MEI FU, Hewlett-Packard Laboratories, QIANG ZHANG, Stanford University, THADDEUS LADD, Stanford University and National Institute of Informatics, Toyko Japan, COLIN STANLEY, H.C. HOLLAND, University of Glasgow, YOSHIIHSA YAMAMOTO, Stanford University and National Institute of Informatics, Toyko Japan — Electron spins bound to neutral donors in GaAs are promising systems for quantum information processes. These electron spins form three-level Lambda-type systems that can be manipulated quickly by ultrafast light pulses and have potentially long storage times, making them natural candidates for quantum information manipulation and storage. Unlike quantum dots, they are extremely homogeneous, making multi-qubit interactions and entanglement more accessible. Here, we report on our efforts to coherently control these electron spins using fast pulses and an all-optical spin-echo technique. Using three, off-resonant, small-angle (pi/3), ultrafast (2 ps) pulses, we have demonstrated that the spins exhibit an echo signal indicating T2 coherence times much longer than the previously measured 1 ns T2* bulk dephasing time. The visibility of the echo signal and the delay gives us insights into the T2 decoherence time and decoherence processes in this system. Currently, we are measuring coherences as long as 4 microseconds.

9:24AM A17.00006 Time-resolved luminescence of hierarchically self-assembled GaAs/AlGaAs quantum dots1, BOTAO ZHANG, University of Pittsburgh, ARMANDO RASTELLI, OLIVER SCHMIDT, Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany, JEREMY LEVY, DAVID SNOKE, University of Pittsburgh, ALBERT HEBERLE, Sullivan Park R&D Center, Corning Incorporated and University of Pittsburgh — Hierarchically self-assembled GaAs/AlGaAs quantum dots are promising building blocks for quantum information processing and novel lasers because they combine the tight confinement of InGaAs dots with the size homogeneity and a shorter emission wavelength of the GaAs/AlGaAs system at which many photodetectors are especially sensitive. So far, the emission dynamics of these structures has been unexplored. With a streak camera connected to a confocal microscope, we have measured the luminescence dynamics after direct optical picosecond excitation into the quantum dot states at a sample temperature of 10 K. Ensembles of high-density quantum dots (30 dots/μm²) with well-separated transitions give information on state filling as well as intra- and interband relaxation. Single quantum dots on low-density samples (0.5 dots/μm²) with microelectroluminescent emission line widths reveal furthermore the time scale of biexciton formation and decay, as well as coherent effects.

1This work is supported by NSF DMR-0605854.
9:36AM A17.00007 Highly-reduced Fine-structure splitting in InAs/InP quantum dots offering efficient on-demand 1.55 µm entangled photon emitter , LIXIN HE, University of Science and Technology of China, M. GONG, C-F LI, G-C GUO. University of Science and Technology of China, A. ZUNGER, National Renewable Energy Laboratory — There has been intense recent interest in finding efficient entangled photon sources, including the demonstration of generation of “event-ready” entangled photon pairs via a biexciton cascade process using an (In,Ga)As/GaAs quantum dot (QD). However, a genuine finite energy difference between photons with different polarizations, known as the fine structure splitting (FSS), can destroy the entanglement of the photon pairs. To achieve entanglement from (In,Ga)As/GaAs QD, it was, indeed, necessary to Cherry-pick a sample with extremely small FSS from a large number of samples, or to apply strong in-plane magnetic field. Furthermore, the emission wavelength of (In,Ga)As/GaAs QD (880 - 950 nm) is mismatched with the 1.55 µm needed for communications using the optical fibers. Using theoretical modeling of the fundamental causes of FSS in QDs, we predict that the intrinsic FSS of InAs/InP QDs is an order of magnitude smaller than that of InAs/GaAs dots, and better yet, their excitonic gap matches the 1.55 µm fiber optic wavelength, therefore offer efficient on-demand entangled photon emitters for long distance quantum communication.

9:48AM A17.00008 Estimation of extrinsic detection efficiency using intrinsic detection sensitivity of the commercial single photon detector, KIYOTAKA HAMMURA, XIULAI XU, FREDERIC BROSSARD, DAVID WILLIAMS, Hitachi Cambridge Laboratory — The detection efficiency (DE) of the commercial single-photon-receiver based on InGaAs gate-mode avalanche photodiode is estimated using the detection sensitivity (DS). Instalment of a digital-blanking-system (DBS) to reduce dark current makes the difference between DS, which is an efficiency of the detector during its open-gate/active state, and the total/overall detection efficiency (DE). By numerical simulations, it is found that the average number of light-pulses, blanked by DBS, following a registered pulse is 0.333. DS is estimated at 0.216, which can be used for estimating DE for an arbitrary photon arriving rate and a gating frequency of the receiver.

10:00AM A17.00009 Quantum key distribution with an unknown and untrusted source, YI ZHAO, BING QI, HOI-KWONG LO, Center for Quantum Information and Quantum Control, Department of Physics and Department of Electrical & Computer Engineering, University of Toronto — The security of a standard bi-directional “plug & play” quantum key distribution (QKD) system has been an open question for a long time. This is mainly because its source is equivalently controlled by an eavesdropper, which means the source is unknown and untrusted. Qualitative discussion on this subject has been made previously. In this paper, we present the first quantitative security analysis on a general class of QKD protocols whose sources are unknown and untrusted. The securities of standard BB84 protocol, weak-cd-vacuum decoy state protocol, and one-decoy decoy state protocol, with unknown and untrusted sources are rigorously proved. We derive rigorous lower bounds to the secure key generation rates of the above three protocols. Our numerical simulation results show that QKD with an untrusted source gives a key generation rate that is close to that with a trusted source. Our work is published in [1].


10:12AM A17.00010 Spectral study of type-0/type-I spontaneous parametric down-conversion in a PPKTP waveguide1, JUN CHEN, AARON PEARLMAN, ALEXANDER LING, ALAN MIGDALL, JINGYUN FAN, Joint Quantum Institute, National Institute of Standards and Technology, and University of Maryland, JOINT QUANTUM INSTITUTE, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, AND UNIVERSITY OF MARYLAND TEAM — Compared with their bulk-crystal counterparts, SPDC in second-order (χ(2)) nonlinear optical waveguides has been used to generate correlated photons that are naturally emitted into a single spatial mode in a collinear geometry, easing the effort in efficient photon collection and leading the potential to make chip-scale devices for quantum-information-processing applications. Here towards building chip-scale devices for quantum-information-processing applications, we performed the first spectral characterization of correlated two-photon, and single-photon emission for both type-0 and type-I spontaneous parametric down-conversion (SPDC) in a periodically-poled KTiOPO4 (PPKTP) waveguide.

1Spectral study of type-0/type-I spontaneous parametric down-conversion in a PPKTP waveguide

10:24AM A17.00011 Deterministic generation of entangled photon pairs from a semiconductor quantum dot, ANDREAS MULLER, WEI FANG, Joint Quantum Institute, NIST and University of Maryland, Maryland, USA, JOHN LAWALL, National Institute of Standards and Technology, Maryland, USA, GLENN SOLOMON, Joint Quantum Institute, NIST and University of Maryland, Maryland, USA — Optical tuning based on the AC Stark effect is used to cancel the fine-structure splitting in a single self-assembled InAs quantum dot. Under this condition, polarization anisotropy vanishes, and photon pairs emitted from the biexcitonic radiative cascade become polarization-entangled. Entanglement is verified by well-known criteria applied to the two-photon density matrix that was reconstructed experimentally via quantum state tomography. Our approach uses a planar optical microcavity for efficient background laser discrimination, and yields triggered polarization-entangled photons deterministically.

10:36AM A17.00012 Indistinguishable photons from independent semiconductor single-photon devices, THADDEUS LADD1, KAORU SANAKA2, Stanford University, ALEXANDER PAWLIS1, KLAUS LISCHKA, University of Paderborn, Germany, YOSHIHISA YAMAMOTO4, Stanford University — We demonstrate quantum interference between single photons generated by the radiative decay processes of excitons that are bound to isolated fluorine donor impurities in ZnSe/ZnMgSe quantum-well nanostructures. Single photon generation is confirmed by auto-correlation experiments, and indistinguishability of single photons from independent devices is confirmed via a Hong-Ou-Mandel dip. These results indicate that donor impurities in appropriately engineered semiconductor structures can portray atom-like homogeneity and coherence properties, potentially enabling scalable technologies for future large-scale optical quantum computers and quantum communication networks.

1also at National Institute of Informatics, Tokyo, Japan
2also at National Institute of Informatics, Tokyo, Japan
3also at Stanford University
4Also at National Institute of Informatics, Tokyo, Japan

Monday, March 16, 2009 8:00AM - 11:00AM — Session A18 SPOLY: Bulk Block Copolymers I
8:00AM A18.00001 Order-order transition among lamellae, $F_{dd}$, and gyroid in diblock copolymer melts, MIKIHIKO TAKENAKA, MYUNG IM KIM, TSUTOMU WAKADA, SATOSHI AKASAKA, SHOTARO NISHITSUJI, KENJI SAJO, HIROKAZU HASEGAWA, Kyoto University, KAZUKI ITO, Riken, KYOTO TEAM, RIKEN TEAM — We firstly found a Disorder-Gyroid-$F_{dd}$-Lamellae transition behavior found poly(styrene-b-isoprene) (S-I) diblock copolymer melts in previous study. In this study, we will present the dynamics of order-order transition (OIT) among lamellae, $F_{dd}$, and gyroid. We investigated the dynamics of OIT by using time-resolved small angle X-ray scattering with Synchrotron radiation X-ray source. We found that $F_{dd}$ structure was formed as a metastable structure during the OIT from lamellae to gyroid induced by temperature jump.

8:12AM A18.00002 Determination of $F_{dd}$ phase boundary in polystyrene-block-polyisoprene diblock copolymer, MYUNG IM KIM, SATOSHI AKASAKA, TSUTOMU WAKADA, MIKIHIKO TAKENAKA, HIROKAZU HASEGAWA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University — We previously reported the discovery of a novel bicontinuous microdomain structure with $F_{dd}$ symmetry in polystyrene-block-polyisoprene (SI) diblock copolymer. In this study, we investigated the phase behavior of eight SI diblock copolymer samples having slightly different compositions ($0.627 \leq f_{PI} \leq 0.653$) by SAXS and TEM to determine the phase boundary of the $F_{dd}$ structure in the phase diagram of SI. The SI having the lowest $f_{PI} (= 0.627)$ showed only disorder-lamella (L) transition but no order-order transition. The SI having the largest $f_{PI} (= 0.653)$ showed disorder-gyroid (G)-L transition with decreasing temperature, but did not show $F_{dd}$ phase. The other six SI samples having $f_{PI}$ values between these two exhibited disorder-G-$F_{dd}$-L transition with decreasing temperature. Consequently, we could determine the compositional region where $F_{dd}$ phase is thermally stable, which is in good agreement with that predicted by SCFT.

8:24AM A18.00003 Stabilization of Bicontinuous Phases in Diblock Copolymer Systems, FERNANDO ESCOBEDO, FRANCISCO MARTINEZ-VERACOECHEA, Cornell University — We used a coarse-grained description of the copolymer chains (i.e., dissipative particle dynamics fluid), together with continuum-space Monte Carlo and Molecular Dynamics methods, to study systems of diblock copolymers melts that have been "filled" with selective additives (i.e., homopolymer, and nanoparticles). Approximate phase boundaries were found via free-energy calculations. We focus on the stabilization of bi-continuous phases and the strikingly different phase behavior observed when the nature of the selective filler is changed. Our results elucidate the origins of the packing frustration that limits the viability of the gyroid, double-diamond, and plumber’s nightmare phases and provide insights for overcoming it. Attention is also focused on directly determining the areas of phase diagram where macro- phase separation occurs. We compare the particle-based simulation results with the results obtained by means of self-consistent filed theory calculations.

8:36AM A18.00004 Structure-Properties Relationship in Proton Conductive Sulfonated Polystyrene-Poly(methacrylate) Block Copolymers, LAURENT RUBATAT, CHAOXU LI, HERVE DIETSCHE, University of Fribourg, Switzerland, ANTTI NYKAINEN, JANNE RUOKOLAİNEN, Helsinki University of Technology, Finland, RAFFAELE MIZZENGA, University of Fribourg, Switzerland — We report on the dependence of proton conductivity on the morphologies of sulfonated polystyrene-poly(methyl methacrylate) (sPS-PMMA) diblock copolymers. Three diblock copolymers of varying molecular weight and block volume fraction were studied, for each one several sulfonation degrees of the PS block were considered. The investigation of the morphologies of the self-assembled sPS-PMMA diblocks was carried out by means of small angle neutron scattering and transmission electron microscopy. Depending on molecular weight and sulfonation degrees, isotropic phase (ISO), lamellar phase (LAM), cylindrical hexagonal phase (HEX) and hexagonally perforated lamellae (HPL) were observed. Proton conductivity, normalized by the volume fraction of the conductive domains (formed by PS, sPS, and water) was shown to rise monotonically with the following sequence of morphologies: ISO to HEX to HPL to LAM.

8:48AM A18.00005 Morphology of Sulfonated Styrenic Pentablock Copolymer Solutions and Membranes, ARUN KOTA, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania — We report a systematic investigation of the morphology of sulfonated styrenic pentablock copolymer solutions and membranes obtained from Kraton Polymers LLC. The polymer studied was poly(f-butyl-styrene)-b-(ethylene-r-butylene)-b-(styrene-r-styrene sulfonate)-b-(ethylene-r-butylene)-b-(f-butyl-styrene). Small angle X-ray scattering (SAXS) revealed that the solutions exhibited micellar morphologies. The solution SAXS data was modeled using the Kinning-Thomas model to obtain radius of the micelle core, the radius of closest approach between two micelles and the volume fraction of micelles. The membranes exhibited anisotropic morphologies with different d-spacings in-plane and through-plane. A good linear correlation was observed between the radius of closest approach between two micelles in the solutions and the d-spacings in the membranes. Efforts are underway to characterize the type of morphology in the membranes using electron microscropy and correlate them to the transport properties.

9:00AM A18.00006 Thermodynamic Behavior of Poly(styrene-b-styrene sulfonate) Block Copolymers With Varying Counterions, KEVIN CAVICCHI, The University of Akron, KEVIN POLLACK, Carleton College — A series of poly(styrene-b-styrene sulfonate) (PS-b-PSS) block copolymers have been prepared by RAFT polymerization. The counterions in the PSS block have been varied by neutralizing the sulfonate groups with alkyl amines or quaternary ammonium ions. The choice of counterion has a strong effect on the lipophilicity of the PSS block. This presentation will focus on the resulting morphology and bulk thermodynamic behavior of these polymers as a function of the PSS concentration. The use of these materials for preparing ion-exchange membranes will be discussed.

9:12AM A18.00007 Salt Doping in PEO Containing Block Copolymers: Counterion and Concentration Effects1, WEN-SHIUE YOUNG, THOMAS EPPS, University of Delaware — Salt-doped poly(ethylene oxide)-based block copolymers are promising candidates for lithium battery electrolytes, which require high ionic conductivities and adequate mechanical integrity. We studied the phase behavior of poly(styrene-b-ethylene oxide) block copolymers doped with various lithium salts over a range of [EO]:[Li] ratios. Small-angle X-ray scattering, transmission electron microscopy, and differential scanning calorimetry experiments were used to characterize the phase behavior of our samples. Specimens were prepared in an argon atmosphere and rigorously dried to reduce the effects of moisture uptake on phase behavior. We found that we can tune the micellar microstructure by varying the lithium counterion as well as the salt doping ratio. Using strong segregation theory, we estimated an effective interaction parameter for the salt-doped copolymers, which varies linearly with salt concentration, where the slope is influenced by the nature of the counterion.

9:24AM A18.00008 Ion transport through block copolymer electrolytes, SCOTT MULLIN, ASHOUTOSH PANDAY, NITASH BALSARA, UC Berkeley — Poly(styrene)-block-poly(ethylene oxide) (SEO) is a candidate material for electrolytes for rechargeable lithium metal batteries. The PS phase suppresses lithium dendrite growth on the anode during recharge, and the PEO phase solvates lithium bis[(trifluoromethane)sulfonimide] salt to form conducting pathways. Complete electrochemical characterization of PEO/LITFSI mixtures requires measurement of conductivity, salt diffusion coefficient, and lithium ion transference number. The present study covers SEO copolymers that exhibit lamellar and cylindrical morphologies in the absence of salt. The addition of salt affects morphology but the relationships between morphology and electrochemical characteristics have not yet been clarified. Some aspects of these relationships will be presented.

1 ACS Grant PRF-46864-67
9:36AM A18.0009 Morphology of Novel Semicrystalline Ethylene-α-Olein Block Copolymers, SHENG LI, RICHARD REGISTER, Princeton University; BRIAN LANDES, Dow Chemical Company — In semicrystalline block copolymers, the solid-state structure can be set either by block incompatibility or by crystallization of one or more blocks. Depending on the block interaction strength, a wide array of solid-state morphologies may be observed, ranging from spherulitic to confined crystallization within preexisting microphase-separated domains. Dow Chemical has recently developed a novel chain shuffling polymerization process to produce olefin block copolymers with alternating amorphous and semicrystalline chain segments, where each block exhibits the most-probable distribution. We examined the melt and solid-state morphologies of these novel olefin block copolymers, having a high octene content in the amorphous block, using two-dimensional synchrotron small-angle and wide-angle x-ray scattering on specimens oriented by channel die compression. Multiblock and diblock copolymers with near-symmetric compositions showed well-ordered lamellar structures at room temperature with long periods exceeding 100 nm, with little dependence on thermal history, indicating the presence of a mesophase-separated melt which templates crystallization.

9:48AM A18.00010 Self-assembly of crystalline bioinspired block copolymers, A.M. ROSALES, H.K. MURREN, Dept. of Chemical Engineering, University of California - Berkeley, R.N. ZUCKERMANN, Molecular Foundry, Lawrence Berkeley National Laboratory, R.A. SEGALMAN, Dept. of Chemical Engineering, University of California - Berkeley — Polypeptides are sequence-specific biologically inspired polymers based on N-substituted glycines for which monodisperse, polymeric molecular weights can be achieved. Sequence control allows for a degree of tunability in both the self-assembly and thermal properties not available in classical polymer systems. We demonstrate that a series of homopolypeptides are thermally stable to 300°C and are crystalline with melting transitions ranging from 150°C to 250°C. The introduction of defects at precise locations in the polymer sequence (as a side chain substitution) allows crystallization and hence the melting temperature to be suppressed. Symmetric block copolymers with two crystalline polyolefin blocks exhibit co-crystallization of the two blocks but distinct melting behaviors, indicating a disordered melt. If samples are carefully prepared to allow for microphase separation, block copolymer lamellae with long range order are formed with an order-disorder transition temperature well below the melting transition temperature of the polymer.

10:00AM A18.00011 Crystallization, Crystal Orientation and Morphology of Poly(ethylene oxide) under 1D Defect-Free Nanoscale Confinement, MING-SIAO HSIAO, The University of Akron; JOSEPH X. ZHENG, RYAN M. VAN HORN, RODERIC P. QUIRK, EDWIN L. THOMAS, MIT; BERNARD LOTZ, Institute Charles Sadron; STEPHEN Z. D. CHENG — One-dimensional (1-D) defect-free nanoscale confinement is created by growing single crystals of PS-b-PEO block copolymers in dilute solution. Those defect-free, 1-D confined lamellae having different PEO layer thicknesses in PS-b-PEO lamellar single crystals (or crystal mats) were used to study the polymer recrystallization and crystal orientation evolution as a function of recrystallization temperature \( T_{rx} \) because the \( T_{PS} \) of PS-b-PEO lamellae is lower than the \( T_{PEO} \) in the PS-b-PEO single crystal. The results are summarized as follows.

10:12AM A18.00012 Gradient Architecture as Means of Phase Diagram Manipulation in Copolymers: Accessing Both LCOT and UCOT in High Molecular Weight Styrene/n-Butyl Acrylate Systems, MICHELLE MOK, WESLEY BURGHARDT, Northwestern University; CHRISTOPHER ELLISON, University of Texas at Austin, JOHN TORKELSON, Northwestern University — Traditionally, phase transitions of block copolymers could only be tuned through molecular weight and relative block length. Here, we introduce comonomer sequence design through gradient compositions as a means of further manipulating phase diagram boundaries. In such gradient copolymers, the reduced repulsion between chain segments allows access to phase transitions even at high molecular weights (MW). Rheological and x-ray scattering studies were performed to study the impact of comonomer sequence on phase behavior in styrene/n-butyl acrylate (S/nBA) systems. In S/nBA block copolymers, only upper critical ordering behavior was observed. In contrast, by using a gradient architecture of higher MW we observed both upper and lower ordering transitions similar to those seen in very weakly segregating S/n-butyl methacrylate block copolymers, where such dual ordering transitions were first detected by Russell et al. This is the first study to access a miscibility gap in gradient copolymers. Access to such behavior is very rare in blends and block copolymers, limited to low MW and/or very weakly segregating systems.

10:24AM A18.00013 Effects of polydispersity on the order-disorder transition of diblock copolymer melts, TOM BEARDSLEY, MARK MATSEN, University of Reading — The effect of polydispersity on an AB diblock copolymer melt is investigated using lattice based Monte Carlo simulations with parallel tempering (PT) techniques. We consider melts where the B blocks are monodisperse and the A blocks are polydisperse with a Schultz-Zimm distribution. Expanding our previous work on polydisperse melts of symmetric composition, we now construct a polydisperse phase diagram, investigating the size of the domains and locations of the order-disorder (ODT) and order-order (OOT) transitions. The PT method has yielded a number of benefits over single-processor temperature scans, including: simulating a number of temperatures simultaneously, annealing out defects in the configurations more readily and capturing the distinctive spike in the heat capacity that occurs at the ODT, allowing the location of the transition to be determined more accurately than in previous studies. The results are compared to those of experiment and to the predictions of self-consistent field theory (SCFT).

We acknowledge the EPSRC (EP/E010342/1) for financial support.

10:36AM A18.00014 Dynamics of Disordered PI-PtBS Diblock Copolymer, HIROSHI WATANABE, Kyoto University — Viscoelastic \( (G^*) \) and dielectric \( (\varepsilon''^*) \) data were examined for a LCST-type diblock copolymer composed of polyisoprene (PI; \( M = 53K \)) and poly(\( \mu \)-tert-butyl styrene) (PtBS; \( M = 42K \)) blocks disordered at \( T \leq 120^\circ\)C. Only PI had the type-A dipole parallel along the chain backbone. Thus, the \( \varepsilon''^* \) data reflected the global motion of the PI block, while the \( G^* \) data detected the motion of the copolymer chain as a whole. Comparison of these data indicated that the PI block relaxed much faster than the PtBS block at low \( T \) and the dynamic heterogeneity due to PtBS was effectively quenched to give a fractional nonuniformity for the PI block relaxation. The \( \varepsilon''^* \) data were thermo–hechoeochemically complex at low \( T \), partly due to this nonuniformity. However, the block connectivity could have also led to the complexity. For testing this effect, the \( \varepsilon''^* \) data were reduced at the iso- frictional state defined with respect to bulk PI. In this state, the \( \varepsilon''^* \) data of the copolymer at low and high \( T \), respectively, were close to the data for the star-branched and linear bulk PI. Thus, the PI block appeared to be effectively tethered in space at low \( T \) thereby behaving similarly to the star arm while the PI block tended to move cooperatively with the PtBS block at high \( T \) to behave similarly to the linear PI, which led to the complexity of the \( \varepsilon''^* \) data. The PtBS block also exhibited the complexity (noted from the \( G^* \) data), which was well correlated with the complexity of the PI block.
10:48AM A18.00015 Morphology of Renewable Polylactide / Soybean Oil Blends Compatibilized by Block Copolymers1, MEGAN ROBERTSON, KWAHNO CHANG, MARC HILLYER, University of Minnesota-Twin Cities — Renewable composites derived from polylactide and soybean oil (soy) were prepared by melt blending. The blend morphology was tuned with the addition of poly(isoprene-b-lactide) block copolymers. Due to the extreme differences in the viscosities of soy and polylactide, a critical block copolymer block ratio was found to induce a phase inversion in which the morphology changed from soy droplets in a polylactide matrix to polylactide droplets in a soy matrix, even though soy was the minority component. This transition was not only due to the thermodynamic interactions between the block copolymer and the two immiscible phases, but also was a result of shear forces acting on the mixture during melt blending. The droplet size of the soy droplets in the polylactide matrix was also highly dependent on the block copolymer composition. In binary polylactide/soy blends there was a limiting concentration of soy which could be incorporated into the polylactide matrix (5 percent of the total blend weight) due to the mismatch in viscosities resulting in the loss of soy during mixing. The addition of block copolymer with an appropriate block ratio allowed full incorporation of soy up to 20 percent of the total blend weight.

1 Funding provided by Toyota Motor Inc.

Monday, March 16, 2009 8:00AM - 11:00AM
Session A19 DPOLY: The Physics of Polymer Nanocomposites: Polymer Nanoparticle Interactions 320

8:00AM A19.00001 Functional polymer colloids stabilized by type-purified single-wall carbon nanotubes, ERIK K. HOBBS, JEFFREY A. FAGAN, JAN OBRZUT, NIST — Emulsion polymerization of a methacrylate monomer in aqueous biological suspensions of type-purified single-wall carbon nanotubes (SWNTs) is used to synthesize polymer colloids coated by nearly pure metallic or semiconducting SWNTs. The polymer-nanocomposite spherical particles are 1-100 micrometers in diameter, are marginally stable in ethanol, and retain the color and unique optical characteristics of the purified SWNT coating in the absence of any surfactant. By assembling these functional polymer colloids on microelectronic circuits, we characterize the electronic properties of the SWNT-polymer nanocomposite microspheres and relate this to the band structure of the purified SWNT coating, demonstrating their potential use as microscopic optical and electronic components that can be easily manipulated using standard methods of colloidal self-assembly.

8:12AM A19.00002 Theoretical analysis of dispersing of aggregated nanorods in shear flow in presence of AC electric or magnetic fields, VICTOR PRYAMITSYN, VENKAT GANESAN, The University of Texas at Austin — Efficient dispersion of nanotubes in polymeric matrices is a critical problem confronting the development of modern polymer nanocomposites. The nanotube-nanotube interactions usually promote aggregation, which also depends on factors such as the chemical makeup of the polymer matrix and the size of nanotubes. High intensity mechanical mixing such shear pulverization are commonly used for dispersion of nanotubes. The main disadvantage of such processes is the degradation of polymer matrix, which may downgrade the final properties of PNC’s. In this work, we theoretically explore a novel strategy to reduce the shear stresses required for dispersion of rod-like fillers. Explicitly, we found that simultaneous applications shear flow and AC electric field oriented at an angle to each other may cause rod rotational instabilities of the rods suspension and lead to the dispersion of the rods. We demonstrate this idea through Brownian dynamics simulations of aggregating nanorods and a complementary theoretical analysis using a 2D Smoluchowski equation. Our results suggest that an optimal dispersion may be achieved at an shear-E field orientation of β = ±45° with an optimal amplitude of AC electric field which is proportional to the rotation Peclet number of nanorods suspension.

8:24AM A19.00003 Effective Interactions, Structure and Phase Behavior of Polymer Nanocomposites with Nonspherical Fillers, LISA M. HALL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — The Polymer Reference Interaction Site Model is applied to study polymer-mediated inter-nanoparticle interactions, fluid structure, and miscibility of nonspherical filler particles in a melt of adsorbing freely-jointed chains. The behavior of hard rod, disk, and cube-like nanoparticles are compared. The depletion contact aggregation, dispersion, and polymer matrix mediated nanocomposite network states of organization are sensitive to filler shape. A detailed study of thin rod fillers, including the rod-rod potential of mean force and second virial coefficient, B2, as a function of polymer-rod and rod-rod attraction strengths, has also been performed. A primary goal is to identify design rules for dispersing nanotubes in polymer melts. Shortening the spatial range of rod-rod attraction compared to polymer-rod attraction increases miscibility. The transition from positive to negative B2 at low polymer-rod interfacial attraction (entropic depletion) occurs more readily (at higher attraction strength) as rod-rod attraction is increased. However, the transition to negative B2 at high polymer-rod attraction strength, driven by polymer-induced enthalpic bridging of rods, is relatively invariant to inter-rod attraction strength. Increasing rod length reduces the stabilizing consequences of polymer adsorption and the attendant steric repulsion.

8:36AM A19.00004 Polymer-tethered nanoparticle “shape amphiphiles”: A new class of macromolecular building block for self-assembly, SHARON GLOTZER, University of Michigan — Fabricating complex ordered structures from nanoparticles requires controlling nanoparticle interactions for self-assembly over multiple length scales. Here we exploit both building block shape and interaction anisotropy for self-assembly, and explore the use of polymer “tails” attached to nanoparticle “head groups” to create a new kind of amphiphile that self assembles into structures like those seen in surfactant and block copolymer systems, but with important differences arising from nanoparticle shape, and tethered nanoparticle geometry and topology. We investigate the impact of nanoparticle size polydispersity and show that it can both help and hinder formation of certain complex phases. Using simulation, we investigate tethered spheres, rods, cubes, triangles, and other shapes, and provide design rules for the predicted self-assembly of a range of chiral and achiral structures, including helical scrolls, gyroid, square arrays, and ionic crystal-like structures.

9:12AM A19.00005 Control of the Spatial Distribution of Nanoparticles in Fluorescent Polymer Nanocomposites1, CHELSEA CHEN, PETER GREEN, University of Michigan, Ann Arbor — In a brush-coated nanoparticle (NP) / polymer nanocomposite system, the spatial distribution of the NPs is largely determined by the entropic and enthalpic interactions between the brush and polymer host chains. We examined the miscibility between polystyrene (PS) homopolymer chains and a fluorescent polymer poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) and found that in thin films, low molecular weight (MW) PS and MEH-PPV are miscible, whereas high MW mixtures exhibit phase separation. Consequences of this behavior were examined with regard to the effect on the morphology of nanocomposite thin films composed of MEH-PPV and thiol terminated polystyrene grafted Au nanoparticles of varying sizes. We were able to achieve complete dispersion, as well as interfacial segregation, of the Au-PS nanoparticles within MEH-PPV hosts. Through control of the morphology, we were able to “tune” the optical properties of the MEH-PPV/Au-PS nanocomposites.

1Supported by DOE#DE-FG02-07ER46412 and NSF#DMR 9871177.
9:24AM A19.00006 Importance of Chain Connectivity in the Formation of Non-covalent Interactions between Polymers and Single-Walled Carbon Nanotubes, DIAS LINTON, BRAD C. MILLER, HUIMIN LI, CHARLES FEIGERLE, Department of Chemistry, University of Tennessee, Knoxville, TN 37996; BOBBY C. SUMPTER, Oak Ridge National Laboratory, Oak Ridge, TN 37831; MARK D. DADMUN, Department of Chemistry, University of Tennessee, Knoxville, TN 37996 and Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Our work is focused on understanding and utilizing non-covalent electron donor-acceptor (EDA) interactions between polymers and SWNT to optimize interfacial adhesion and homogeneity of nanocomposites without modifying the SWNT native surface. Nanocomposites with polymer bound electron donating or withdrawing moieties leads to improved SWNT dispersion if the interacting functional group is a minor component of a copolymer matrix. Correlation of experimental (Raman mapping, Raman D* band peak shifts, and optical microscopy) and computational results indicates that chain connectivity is critical in controlling the accessibility of the functional groups to form EDA interactions. Thus, controlling the amount of e-donating or withdrawing moieties throughout the polymer chain will direct the extent of EDA interaction, which enables tuning the SWNT dispersion.

9:36AM A19.00007 The Structure of Amphiphilic Polymers Interacting with Carbon Nanotubes, YACHIN COHEN, MEIRAV GRANITE, Technion, Israel, WIM PYCKHOUT-HINTZEN, AUREL RADULESCU, Fz. Juelich, Germany — Dispersion of single-walled carbon nanotubes, necessary for their beneficial utilization, is often based on amphiphilic copolymers. We have successfully utilized the following systems: an alternating copolymer of styrene and sodium maleate, exhibiting alternating hydrophobic and hydrophilic groups, amphiphilic block copolymers such as Pluronic F108 and a synthetic short polypeptide (FFDD), containing alternating hydrophobic blocks of two phenylalanine (FF) and hydrophilic block of two aspartic acid (DD). Cryo-transmission electron microscopy images reveal isolated, very small bundles of carbon nanotubes, with diameters range from 1 to 5 nm and approximately 500 nm length. Small-angle neutron scattering experiments were conducted at different D$_2$O/H$_2$O content of the dispersing medium. The scattering patterns suggest a complex entity with an heterogeneous structure. For the alternating copolymer, loose adsorption of polymer coils is indicated, contrary to published ideas on “polymer wrapping” of nanotubes. For the Pluronic block copolymers, the data suggest that even below the critical micellization temperature there is a dense coating on the nanotube surface and the hydrophilic blocks are highly extended. The polypeptide also forms a dense coating with an apparently “spongy” structure.

9:48AM A19.00008 Chain Expansion in Polymer-Nanoparticle Melts, A. L. FRISCHKNECHT, Sandia National Laboratories, E. S. MCGARRITY, Michigan State University, M. E. MACKAY, University of Delaware — We apply a self-consistent version of the polymer reference interaction site model (PRISM) theory to a model of spherical nanoparticles in a polymer melt. The average radius of gyration of the chains in the blend clearly increases (over that from chains in a neat melt at the same density) with increasing nanoparticle volume fraction. The amount of chain expansion also depends on the magnitudes of the attractive interactions in the system. The bulk modulus of the blend decreases with increasing nanoparticle volume fraction. We compare our theoretical results to experimental scattering data from polystyrene blends with various nanoparticles and to previous simulation results. (This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.)

10:00AM A19.00009 Effects of nanoparticles on chain dynamics and glass transition in amorphous polymer nanocomposites$^1$, HYUN JOON OH, PETER GREEN, University of Michigan, Ann Arbor — Chain relaxation dynamics and the glass transition of mixtures of polystyrene (PS) homopolymer with PS-grafted gold nanoparticles were examined using broadband dielectric spectroscopy, differential scanning calorimetry and capacitive scanning dilatometry. Through changes in the nanoparticle core size, $D$, grafting density, $g$, degree of polymerization of grafted chains, $N$, and the nanoparticle concentration, $\phi$, both the chain relaxation time, $\tau$, and the $T_g$ could be induced to undergo significant changes, increases or decreases, in magnitude. These results will be discussed in light of dynamics in other polymer/nanoparticle systems. In addition, the role of particle size and the role of the melt/brush interfacial interactions on the dynamics will be discussed.

$^1$Work supported by the US DOE (DE-FG02-07ER46412) and by the NSF (DMR-0601890).

10:12AM A19.00010 Dynamics in Nanoparticle Liquids, PETER MIRAU, AFRL/RXBN, Air Force Research Lab, BioNano Branch, Wright-Patterson AFB, OH 45433, MICHAEL JEPSEN, RICHARD VAIA, AFRL/RXBN, ROBERT RODRIGUEZ, EMMANUEL GIANNELIS, Materials Science & Engineering, Cornell University, Ithaca, NY 14853 — Nanoscale Ionic Materials (NIMS) are organic-inorganic hybrids in which a nanometer-sized core is functionalized with a covalently attached corona and an ionically tethered canopy, NIMS can be engineered to be liquids at ambient temperature in the absence of solvent and are of interest for a variety of applications. We have used NMR relaxation and pulse-field gradient NMR to measure the dynamics of NIMS made from a 20 nm silica core modified with propyl sulfonic acid groups and amino-terminated ethylene oxide/proplylene oxide block copolymers. Carbon NMR studies show that the block copolymer canopy is quite mobile both in the bulk and the nanoparticle liquid. The carbon spin-lattice relaxation times as a function of temperature are fit to a model with rapid librational motions and slower reorientation of the copolymer. Neither the correlation times for reorientation of the block copolymer nor the self-diffusion coefficient are influenced by the presence of the silica nanoparticle core. These data suggest that the liquid-like behavior in NIMS is due to rapid exchange of the block copolymer canopy between the ionically modified nanoparticles.

10:24AM A19.00011 Hierarchically Structured Block Copolymer \ Silicate Nanocomposites, ROSS BEHLING, ERIC COCHRAN, Iowa State University — In this contribution we functionalized MMT with a bromine terminated alkylamine and subsequently polymerized polystyrene-b-(tert-butyl acrylate) via graft-from atom transfer radical polymerization. Hierarchical assembly of these composites was facilitated through targeted graft density, polymer block size, and MMT intrinsic properties. The high graft density on the MMT surface results in confinement effects which force growing polymer chains into highly extended conformations. Block copolymer (BCP) brushes were chosen because they inherently offer an easily tunable method for producing self-assembled structures on the order of tens of nanometer. Montmorillonite (MMT) in its raw state is composed of negatively charged tactoids ranging 100-300 nm in diameter and 2 nm thick. BCP nanocomposites particles arranged under shear into structures spanning several hundreds of nanometers. The equilibrium structures were influenced by the MMT platelet curvature and the BCP interaction parameter, $\chi$. BCP nanocomposites were observed via transmission electron microscopy to display novel morphologies with multiple systems exhibiting interpenetrating networks reminiscent of “worm micelles.”

10:36AM A19.00012 Effect of Copolymer-Nanoclay Interactions on Intercalation Kinetics$^1$, LOAN VO, HARIS RETSOS, EMMANUEL GIANNELIS, Cornell University — We use X-ray diffraction to measure the melt intercalation kinetics of a series of surface-modified clay nanoparticles (nanoclay) with styrene-butadiene-rubber (SBR). Since SBR is a copolymer, both the styrene and the butadiene components interact with the nanoparticles contributing to the nanoclay miscibility and the intercalation kinetics. We are able to directly measure the butadiene-nanoclay interaction strength by using dielectric relaxation spectroscopy to probe the butadiene-nanoclay interfacial relaxation mode, and by varying the nanoclay surfactant and copolymer composition, we can indirectly measure the styrene-nanoclay interaction strength. We will present the spectroscopy results and discuss the relation to the intercalation kinetics.

$^1$Michelin
We gratefully acknowledge funding from the National Science Foundation (DMR 0606086, CBET-0609087) and Petroleum Research Fund (46204-AC7).
oscillations decay exponentially with increasing temperature, as found in studies of the temperature dependence of microwave-induced resistance oscillations in a high-mobility two-dimensional electron system. We find that the systems display overshoots.

In a viscoelastic matrix, however, these overshoots do not appear for 3D drop computations. In this work, we investigate why drop simulations in 3D do not overshoot in the transient evolution of drop deformation. Experimental observations also show that an overshoot can occur when a Newtonian drop is sheared and the viscous shear balance out the interfacial tension force. When a viscoelastic drop is sheared in a Newtonian matrix, numerical simulations exhibit an overshoot, producing a viscoelastic "wake" at the interface at the front and back of the drop. In the case of a drop reaching a stationary state, the stresses in the wake scales with the inverse magnetic field. This observation suggests that the temperature dependence originates primarily from the modification of the single particle lifetime, likely through electron-electron interaction effects. The relevance of our findings to existing theories will be discussed.

This work is supported by NSF DMR-0548014.

10:12AM A20.00010 Newtonian drop deformation in a viscoelastic matrix under shear

10:12AM A21.00002 Temperature dependence of Hall-field induced resistance oscillations in 2D electron systems

Monday, March 16, 2009 8:00AM - 11:00AM –
Session A21 FIAP: Semiconductors: 2D Electrons and Transport 323

8:00AM A21.00001 Temperature dependence of microwave photoresistance in 2D electron systems

8:12AM A21.00002 Temperature dependence of Hall-field induced resistance oscillations in 2D Electron Systems

8:24AM A21.00003 Non-linear transport in microwave-irradiated 2D electron systems at the cyclotron resonance subharmonics

1 This work is supported by NSF DMR-0548014.
8:36AM A21.00004 Observation of Fractional Microwave-Induced Resistance Oscillations using Co-Planar Waveguide on High-Mobility 2DES. KRISTIAN STONE, RUI-RUI DU, Rice University, LOREN PFEIFFER, KEN WEST, Bell Laboratories, Alcatel-Lucent — The microwave-induced resistance oscillations (MIRO) are commonly observed in high-mobility GaAs 2D electron systems (2DES) irradiated by microwaves. Usually this is accomplished using an antenna or waveguide, where the electromagnetic components (E, and H) coincide with the 2DES plane. We explore MIRO in a co-planar waveguide (CPW) geometry, in which E, is the dominant excitation component in the 2DES plane. Our samples are Hall bars of high-mobility, μ= (6 - 12) x10^6 cm²/Vs, GaAs/AlxGa1-x,As quantum wells with electron densities ranging from 3 to 5 x10^11 cm⁻². Microwaves from a tunable source (2 - 40 GHz) were fed in, via a semi-rigid coax cable, to an impedance-matched CPW across the length of the Hall bar, and brought out via a similar semi-rigid coax to a power sensor. Using this CPW geometry, we are able to simultaneously measure the photocconductivity and the microwave transmission across the sample. In a temperature range of 2.0 K - 5.0 K, we observed fractional MIRO associated with ε = 1/2, 1/3, 1/4, and 1/5, where ε = ω/ωc, and ωc is the cyclotron frequency. Experimental data as well as a brief discussion will be presented. The work at Rice was funded by NSF DMR-0706634.

8:48AM A21.00005 Photoconductivity of a 2D electron gas at large filling factors. IVAN DMITRIEV, Karlsruhe, Germany, MAXIM KHODAS, Brookhaven National Laboratory, A.D. MIRLIN, D.G. POLYAKOV, Karlsruhe, Germany, MAXIM VAVILOV, Wisconsin, Madison, USA — We study non-equilibrium dc conductivity of a 2D electron gas, placed in a classically strong perpendicular magnetic field in the presence of in-plane microwave field and generic Gaussian disorder potential. Focusing the consideration on the bilinear response in the microwave field, we identify four different mechanisms essential for the linear dc resistance. We employ two specific models of the disorder relevant for ultra-high-mobility samples and show that the relative strength of the above mechanisms strongly depends on the spatial range of the disorder potential. In particular, when large angle scattering dominates the transport and temperature is sufficiently high, the contribution of the “displacement” mechanism can overcome the “inelastic” contribution, which is dominant at low temperature. For smooth disorder, characterized by small angle scattering, the “displacement” contribution is strongly suppressed. Other contributions are responsible for the microwave-induced corrections to the non-diagonal part of the conductivity tensor and only weakly depend on the nature of the disorder. We discuss the ways to distinguish experimentally the contributions of the above mechanisms according to their different polarization and temperature dependence.

9:00AM A21.00006 Warming in systems with discrete spectrum: spectral diffusion of two dimensional electrons in magnetic field. SERGEY VITKALOV, NATALIA ROMERO KALMANOVITZ, The City College of New York, USA, ALEXEY BYKOV, Institute of Semiconductor Physics, 630000 Novosibirsk, Russia — Warming in complex physical systems, in particular global warming, attracts significant contemporary interest. It is essential, therefore, to understand basic physical mechanisms leading to overheating. It is well known that application of an electric field to conductors heats electric charge carriers. Often an elevated electron temperature describes the result of the heating. This paper demonstrates that an electric field applied to a conductor with discrete electron spectrum produces a non-equilibrium electron distribution, which cannot be described by temperature. Such electron distribution changes dramatically the conductivity of highly mobile two-dimensional electrons in a magnetic field, forcing them into a state with a zero differential resistance. Most importantly the results demonstrate that, in general, the effective overheating in the systems with discrete spectrum is significantly stronger than the one in systems with continuous and homogeneous distribution of the energy levels at the same input power.

2This work was supported by NSF: DMR 0349049 and RFBR, project No.08-02-01051

9:12AM A21.00007 Effect of parallel magnetic field on the zero-differential resistance state. NATALIA ROMERO, SEAN MCHUGH, MYRIAM P. SARACHIK, SERGEY A. VITKALOV, Physics Department, CCNY, A. A. BYKOV, Institute of Semiconductor Physics, Novosibirsk — The non-linear zero-differential resistance state (ZDRS) that occurs for highly mobile two-dimensional electron systems in response to a dc bias in the presence of a strong magnetic field applied perpendicular to the electron plane is suppressed and disappears gradually as the magnetic field is tilted away from the perpendicular at fixed filling factor ν. Good agreement is found with a model that considers the effect of the Zeeman splitting of Landau levels enhanced by the in-plane component of the magnetic field.

3This work was supported by NSF grant DMR 0349049, U. S. DoE grant DOE-FG02-84-ER45153 and RFBR project No.06-02-16869.

9:24AM A21.00008 Magnetoresistance of two-dimensional electrons in Si/SiGe quantum wells in in-plane magnet field at 20 mK. T. M. LU, L. SUN, D. C. TSUI, S. LYON, Princeton University, W. PAN, Sandia National Laboratories, M. MUHLBERGER, F. SCHAFFLER, Universitat Linz, Austria, J. LIU, Y.H. XIE, University of California at Los Angeles — We have measured the magnetoresistance of two-dimensional electrons in two modulation-doped Si/SiGe quantum wells in an in-plane magnetic field at 20mK. It was found that the ratio of the saturation resistance in high in-plane magnetic field to the zero-magnetic-field resistance is dependent on the electron density. At high electron density, the ratio is approximated 1.8. As the electron density decreases and is close to the metal-insulator transition, the ratio is strongly enhanced and appears diverging at a sample dependent characteristic density. The field at which the magnetoresistance saturates as a function of density is linear at high density. It deviates from this linear dependence and appears to extrapolate to zero when the electron density is below ~0.7 x10¹¹/cm².

9:36AM A21.00009 Electron and Hole Transport in 40 MilliKelvin Germanium < 100 >. KYLIE SUNDQVIST, University of California, Berkeley, CRYOGENIC DARK MATTER SEARCH COLLABORATION — Ultrapure germanium at milliKelvin temperatures presents a charge transport regime which is rarely encountered. In this case, thermal phonons play a negligible role and the scattering of electrons and holes is dominated by spontaneous phonon emission. As these carriers are always hot, typical assumptions of thermal equilibrium are no longer valid. Furthermore, for fields of only a few V/cm, the emission of optical and intervalley phonons is highly inelastic such that carrier distributions may differ substantially from the form of a displaced Maxwellian. We present simulation results of transport processes of carriers in germanium < 100 > at a temperature of ≈40 mK. These studies were performed in order to provide a deeper understanding of processes occurring in detectors of the Cryogenic Dark Matter Search (CDMS), which seeks to detect weakly-interacting massive particles (WIMPs) in the halo of our galaxy. As CDMS measures both the ionized charge and the energy in non-thermalized phonons created by particle interactions, we will describe the applicability of these transport simulation results to a wide variety of measured phenomena.

1Funded by the NSF and DOE.
9:48AM A21.00010 Magnetotransport in Zener Tunneling Regime in a High-Mobility Two-Dimensional Hole System. YANHUA DAI, ZHUOQUAN YUAN, CHANGLI YANG, R.R. DU, Rice University, M. J. MANFRA, L. N. PFEIFFER, K. W. WEST, Bell Laboratories, Alcatel-Lucent — Magnetotransport in two-dimensional electron systems (2DES) under a DC-current bias has recently revealed a number of interesting phenomena, including current-induced Zener oscillations [1] and current-induced spin-polarization in Rashba 2DES. We have measured the DC-current induced magnetotransport in high-mobility 2D holes in a C-doped (100) GaAs/Al0.3Ga0.7As quantum well (QW). The QW has a width of 15 nm and a carrier density \( n \sim 2 \times 10^{11} \text{cm}^{-2} \) and a mobility \( \mu \sim 7 \times 10^{5} \text{cm}^{2} / \text{Vs} \) at \( T = 300 \text{ mK} \). We observe sharp features in the differential resistance, which we interpret as Zener tunneling peaks and valley associated with the commensuration transition of Landau orbits. In a gated Hall bar we are able to tune the carrier density to \( n > 2.6 \times 10^{15} \text{cm}^{-2} \) and observe strong positive magnetoresistance, which can be attributed to the inter-subband scattering with light holes. We will discuss the role of electron-electron scattering in the Zener oscillations observed in electron and hole systems. The work at Rice was supported by NSF DMR-0706634. [1] C. L. Yang et al, Phys. Rev. Lett. 89, 076801 (2002).

10:00AM A21.00011 Strongly Temperature-dependent Compressibility of Dilute 2D Holes near the Metal-Insulator Transition. XUAN GAO, Case Western Reserve Univ, NAOTO MASUHARA, GREG BOEBINGER, National High Magnetic Field Lab, LOREN PFEIFFER, Bell Labs, Alcatel-Lucent — We used the capacitance measurement to study the compressibility of dilute 2D holes in a 10nm wide GaAs quantum well for \( T \sim 0.01-0.7 \text{K} \). The sample exhibits the \( B=0 \) metal-insulator transition (MIT) at a critical density \( p_{\text{c}} \sim 1.0 \times 10^{10} \text{cm}^{-2} \). Deep in the metallic state, the sample capacitance decreases slowly as hole density \( p \) increases, due to the (negative) exchange contribution to the compressibility of an interacting 2D system. As \( p \) is reduced below \( p_{\text{c}} \) at low-\( T \), the capacitance of sample diminishes rapidly as a result of the incompressible nature of the insulator state, similar to previous studies (Dultz and Jiang, PRL 84, 4689 (2000); Allison et al., PRL 96, 216407 (2006)). On the other hand, we found that temperature has a strong effect near the MIT, in contrast to literature. In our system, the compressibility of insulator state increases with \( T \) and remains positive, while the behavior of metallic phase is more complex. Notably, for metallic phase with \( p \) slightly above \( p_{\text{c}} \), the sign of compressibility can change from positive to negative as \( T \) increases. This strongly \( T \)-dependent compressibility is possibly related to the competition between two phases with distinctive compressibility in our system, which is more strongly interacting than samples studied previously.

10:12AM A21.00012 Branched flow and caustics in random media with magnetic fields. JAKOB METZGER, RAGNAR FLEISCHMANN, THEO GEISEL, Max-Planck-Institute for Dynamics and Self-Organization and University of Goettingen, Germany — Classical particles as well as quantum mechanical waves exhibit complex behaviour when propagating through random media. One of the dominant features of the dynamics in correlated, weak disorder potentials is the branching of the flow. This can be observed in several physical systems, most notably in the electron flow in two-dimensional electron gases [1], and has also been used to describe the formation of freak waves [2]. We present advances in the theoretical understanding and numerical simulation of classical branched flows in magnetic fields. In particular, we study branching statistics and branch density profiles. Our results have direct consequences for experiments which measure transport properties in electronic systems [3].

10:24AM A21.00013 Possible competing ground states in high mobility electron-hole bilayers. K. DAS GUPTA, A.F. CROXALL, C.A. NICOLL, M. THANGARAJ, H.E. BEERE, I. FARRER, D.A. RITCHIE, M. PEPPER, Cavendish Laboratory, University of Cambridge — Recently it has become possible to fabricate independently contacted high mobility electron-hole bilayer (EHLB) with densities \(< 5 \times 10^{10} \text{cm}^{-2} \) and a separation 10-20 nm in a GaAs/AlGaAs system. In these EHLBs the interlayer interaction can be stronger than the intralayer interactions. Exciton superfluidity in such EHLBs was first predicted almost forty years ago. Since then theoretical works have indicated the possibility of a very rich phase diagram, containing a superfluid, charge density waves, Wigner crystals and a BCS-BEC crossover. However this system has been extremely difficult to fabricate in practice. Very recent experiments have revealed novel features in the interlayer scattering (Coulomb drag) below \( \sim 1 \text{K} \). The Coulomb drag shows strong non-monotonic deviations from a \( T^2 \) behaviour expected for Fermi-liquids at low temperatures. Simultaneously an insulating behaviour in the single layer resistances also appears in both layers inspite of electron mobilities \( > 10^8 \text{cm}^2 / \text{Vs} \text{T}^{-1} \) and hole mobilities \( > 10^5 \text{cm}^2 / \text{Vs} \text{T}^{-1} \). The experimental results may indicate a competition between an excitonic ground state and charge-density waves. [J. Keogh et al / APL, 87,202104 (2005), A.F. Croxall et al arXiv:0807.0117 (to appear in JAP), A.F. Croxall et al arXiv:0807.0134v3 (to appear in PRL)].

10:36AM A21.00014 Anomalous plateau formation and improved quantization in charge pumping under a perpendicular magnetic field. SAMUEL WRIGHT, Cavendish Laboratory and Toshiba Cambridge Research Laboratory, MARK BLUMENTHAL, Cavendish Laboratory and National Physical Laboratory, GODFREY GUMBS, Institute of Molecular and Atomic Physics of the City University of New York, ADAM THORN, MICHAEL PEPPER, Cavendish Laboratory, T.J.B.M. JANSEN, National Physical Laboratory, STUART HOLMES, Toshiba Cambridge Research Laboratory, DAVE ANDERSON, GEB JONES, CHRISTINE NICOLL, DAVE RITCHIE, Cavendish Laboratory — We present experimental results of high frequency quantized charge pumping through a quantum dot formed by the electric field arising from applied voltages in a GaAs/AlGaAs system in the presence of a perpendicular magnetic field \( B \). Improved quantization and robustness in gate voltage are seen as \( B \) is increased. Under application of even higher \( B \) fields, the formation of anomalous plateaux in the pumped current are seen.

10:48AM A21.00015 Thermal transport size effects in self-assembled Germanium quantum dots in single-crystal silicon. JEAN-NUMA GILLET, University of Colorado at Boulder — Superlattices with low thermal conductivity have been used to design 1-D thermoelectric materials. With them, it is challenging to obtain a thermoelectric figure of merit \( ZT > 1 \). Self-assembly is used to fabricate Ge quantum-dot (QD) arrays. High \( ZT \) is expected in these self-assembled Ge QDs arrays in Si since they are single crystals. We prove that high-density 3-D Ge QD arrays in diamond-cubic Si exhibit low thermal conductivity. This property can be used to design 3-D thermoelectric devices. To study the thermal behavior of these 3-D nonphononic crystal nanocomposites, we create an atomistic model of a supercell consisting of Si unit cells. Inside each supercell, we substitute Si atoms with Ge atoms to form a QD. The thermal conductivity has been shown to reduce below 0.2 W/m/K. Such a result is realized by ensuring minimum group velocities. Further reduction is expected from multiple scattering. We are concerned with the size dependence of the thermal conductivity upon the Ge volumic composition \( f \). From preliminary results with constant \( f \), we obtain an exponential-like thermal-conductivity decrease when the supercell size is increased.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A22 GMAG DMP FIAP: Focus Session: Spins in Group III-V and II-VI Semiconductors
8:00AM A22.00001 Electrically Injected Spin Polarized Lasers1 . PALLAB BHATTACHARYA, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, MI 48109-2122, USA — The ability to electrically modulate orthogonal polarization states in spin-polarized lasers opens up avenues for a wide range of applications such as photochemical spectroscopy, optical switches, and communications with enhanced security [1]. This has motivated us to investigate the properties of quantum well (QW) [2] and quantum dot (QD) [3] spin-polarized vertical cavity surface emitting lasers (spin-VCSELs). The laser heterostructures are grown by molecular beam epitaxy (MBE). The active region consists of In0.2Ga0.8As/GaAs QWs [2] or InAs QDs [3]. VCSELs are fabricated using standard micro-fabrication techniques. The FM Schottky tunnel contact is realized with Fe or MnAs re-grown by MBE. The QW spin-VCSELs exhibit a maximum threshold current reduction of 11 % and output degree of circular polarization of 23 % at 50 K. The corresponding values observed in QD spin VCSELs at 200 K are 8 % and 14 %, respectively. Inhibition of the D’yakonov-Perel spin scolding process results in higher operating temperatures for spin-lasers with QD active region. In addition, we have demonstrated electrical modulation of the output polarization with a peak modulation index of 0.6. The spin polarization of carriers in the active region of a spin laser gives rise to large gain anisotropy at biases near threshold. As a result, the output polarization can be much larger than the spin polarization of the injected carriers. This is contrary to the linear relation between carrier spin orientations in the active region and the polarization of photons emitted upon their radiative recombination in spin light emitting diodes. The exact magnitude of the output polarization in spin lasers and the parameters upon which it depends have been analytically determined and are in excellent agreement with those obtained from measurements. These results will be described and discussed.

References:

1 Work supported by the Office of Naval Research.

8:36AM A22.00002 Electrical Spin injection from Fe into ZnSe . AUBREY HANBICKI, G. KIOSEOGLOU, M.A. HOLUB, O.M.J. VAN ’T ERVE, B.T. JONKER, Naval Research Laboratory — The wide bandgap semiconductor ZnSe is an opto-electronic material with a comparable spin lifetime and small lattice mismatch to GaAs. Novel spintronic devices that incorporate ZnSe/GaAs heterostructures will require the facile transport of spin information across several heterointerfaces including spin injection into the ZnSe. We have electrically injected spin-polarized electrons from a ferromagnetic Fe contact into a ZnSe epi layer grown on a GaAs heterostructure. The injected carriers proceed through 300 nm of ZnSe and recombine in the GaAs emitting light characteristic of the bulk GaAs exciton. We measure spin polarizations in excess of 40% in the GaAs based on analysis of the circular polarization of the electroluminescence. We report results as a function of applied magnetic field, device current and temperature. The spin injection process and transport through the ZnSe layer sustains significant spin populations in this heterostructure. This work was supported by core programs at NRL.

8:48AM A22.00003 Tuning spin-current across a Semiconductor/Ferromagnet junction by resonance tunneling , PENGKE LI, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York, 14627, HANAN DERY, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York 14627 — We present a theory of spin-dependent transport in a hybrid semiconductor/ferromagnet system which includes an asymmetric double barrier region at the interface (e.g., GaAs/AlGaAs/GaAs/Fe). The system has two electron confinement regions with one being a thin quantum well between a heterostructure barrier and a Schottky barrier. The second confinement region is a two dimensional electron gas (2DEG) at the heterointerface with the bulk semiconductor generated by intentional doping. The I-V curve has two current peaks when electrons tunnel into the ferromagnet. These peaks are due to resonance tunneling of electrons whose energy matches the energy of the quasi-bound state in the quantum well. The first peak is governed by tunneling of delocalized electrons from the bulk semiconductor and the second by escape from the 2DEG. These resonances are met at different bias levels and correspond to opposite spin polarization of the current.

9:00AM A22.00004 Triggering phase-coherent spin packets by pulsed electrical spin injection across an Fe/GaAs Schottky barrier1 . B. BESCHOTEN, L.R. SCHREIBER, C. SCHWARK, G. GUENTHERODT, Physikalisches Institut II A, RWTH Aachen University, 52056 Aachen, Germany, C. ADEL Mann, C.J. PALMSTROM, Department of Chemical Engineering and Material Science, University of Minnesota, Minneapolis 55455, X. LOU, P.A. CROWELL, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455 — The precise control of spins in semiconductor spintronic devices requires an electrical means for generating spin packets with a well-defined initial phase. So far, ultrafast laser pulses have successfully been used to trigger the ensemble phase of optically generated spin packets. However, electrical methods for ensemble phase triggering remain challenging. Here, we use fast current pulses to inject phase triggered electron spin packets across an Fe/GaAs Schottky barrier into n-GaAs. We demonstrate phase coherence by the observation of multiple Larmor precession cycles for current pulse widths down to 500 ps at 20 K. We show that the current pulses are broadened by the charging and discharging time of the Schottky barrier. At high frequencies, the observable spin coherence is limited only by the finite band width of the current pulses, which is on the order of 2 GHz.

1 Work supported by BMBF, HGF, and by DFG. Work at Minnesota supported by ONR, NSF NNIN and by MRSEC programs.

9:12AM A22.00005 The importance of Fe interface states for ferromagnet-semiconductor based spintronic devices . ANTHANASIOS CHANTIS, Theoretical Division, Los Alamos National Laboratory — I present our recent theoretical studies of the bias-controlled spin injection, detection sensitivity and tunneling anisotropic magnetoresistance in ferromagnetic-semiconductor tunnel junctions. Using first-principles electron transport methods we have shown that Fe 3d minority-spin surface (interface) states are responsible for at least two important effects for spin electronics. First, they can produce a sizable Tunneling Anisotropic Magnetoresistance in magnetic tunnel junctions with a single Fe electrode. The effect is driven by a Rashba shift of the resonant surface band when the magnetization changes direction. This can introduce a new class of spintronic devices, namely, Tunneling Magnetoresistance junctions with a single ferromagnetic electrode that can function at room temperatures. Second, in Fe/GaAs(001) magnetic tunnel junctions they produce a strong dependence of the tunneling current spin-polarization on applied electrical bias. A dramatic sign reversal within a voltage range of just a few tenths of an eV is found. This explains the observed sign reversal of spin-polarization in recent experiments of electrical spin injection in Fe/GaAs(001) and related reversal of tunneling magnetoresistance through vertical Fe/GaAs/Fe trilayers. We also present a theoretical description of electrical spin-detection at a ferromagnet/semiconductor interface. We show that the sensitivity of the spin detector has strong bias dependence which, in the general case, is dramatically different from that of the tunneling current spin-polarization. We show that in realistic ferromagnet/semiconductor junctions this bias dependence can originate from two distinct physical mechanisms: 1) the bias dependence of tunneling current spin-polarization, which is of microscopic origin and depends on the specific properties of the interface, and 2) the macroscopic electron spin transport properties in the semiconductor. Our numerical results show that the magnitude of the voltage signal can be tuned over a wide range from the second effect alone and thus identifies a universal method for enhancing electrical spin-detection sensitivity in ferromagnet/semiconductor tunnel contacts.
9:48AM A22.00006 Three Terminal Spin Extraction Resistance in Fe/GaAs Heterostructures, E.S. GARLID1, T. KONDO1, Q. HU1,2, C.J. PALMSTROM1,2, P.A. CROWELL1, U. Minnesota, 2UC Santa Barbara — Spin transport measurements have been difficult to interpret in two terminal Fe/GaAs/Fe devices where current flows in both the injector and detector electrodes. This is due to the strong non-monotonic dependence of the spin accumulation on the Fe/GaAs interface bias, which affects the spin injection and detection efficiencies. To address this, we measured the four terminal non-local spin valve resistance and the three terminal spin extraction resistance in epitaxial Fe/GaAs heterostructures with a systematically varied Schottky barrier doping profile. Lateral devices were fabricated from epitaxial Fe/n+n-GaAs (100) heterostructures in which the thickness of the n+ layer (n+ = 5 × 1017 cm−2) was varied from 5 to 50 nm while n = 5 × 1016 cm−2 in the 2.5 µm channel. The three terminal resistance measured using a single contact as the injector and detector is ~100× larger than the non-local spin valve resistance, an effect which cannot be attributed to spin relaxation in the channel. In the case of a three terminal measurement, we obtain both a large spin accumulation as well as an enhanced detection sensitivity under forward bias conditions. This can be analyzed by considering the measured non-local spin polarization as a function of bias, as well as the electric fields at the Fe/GaAs interface in the presence of a charge current. Supported by ONR and the NSF MRSEC, and NNIN programs.

10:00AM A22.00007 Contributions to oblique Hanle linewidths in Fe/GaAs non-local spin valve transport, CHAFFRA AWO-AFFOUDA, O. M. J. VAN ‘T ERVE, G. KIOSEOGLOU, A. T. HANKBICKI, M. HOLUB, C. H. LI, B. T. JONKER, Naval Research Laboratory — The transport Hanle effect linewidth is commonly used to determine spin lifetimes in spin- polarized transport structures. We show that the magnetic domain structure of the ferromagnetic contacts used to inject and detect the spin current introduces asymmetries to the Hanle linewidth. In addition, the nuclear spin polarization can produce anomalous narrowing and broadening of the Hanle linewidth depending upon the orientation of the transport spin and the applied field. These contributions can significantly impact the apparent spin lifetime extracted from the Hanle curve, but are not included in the analysis typically applied.

10:12AM A22.00008 High Optical Polarization from Electrical Spin Injection into a InGaAs QW, CH. LI, G. KIOSEOGLOU, M. HOLUB, O.M.J. VAN ’T ERVE, B.T. JONKER, Naval Research Lab, T. ALI, I. KHAN, M. YASAR, A. PETROU, SUNY Buffalo — We have fabricated spin light emitting diodes (LEDs) with Fe as the spin injector and 100 ˚A In0.1Ga0.9As/GaAs QWs as the detector. The emission efficiency from the InGaAs QW is extremely high, with a narrow linewidth of 4meV at 5K. The free exciton exhibits 25% optical polarization due to the injection of spin-polarized carriers from the reverse-biased Fe Schottky contact. At low bias, a feature 10meV below the free exciton appears which exhibits a much larger polarization with a peculiar magnetic field dependence. Similar to that of the free exciton, the circular polarization of this lower energy feature first increases with magnetic field, and reaches a maximum of 67% at 2.5T, indicating injection from Fe. However, this behavior is superposed on a large diamagnetic background of 21%/T which dominates above 2.5T. The intensity and polarization of this feature is strongly bias dependent, and the feature disappears above 15K, suggesting that it originates from a weakly bound complex. The origin of this feature and its dependence on the magnetic field will be discussed at the meeting. Supported by ONR, NRL core funds, and NSF.

10:24AM A22.00009 Spin polarization control through resonant states in an Fe/GaAs Schottky barrier, ATSUFUMI HIROHATA, University of York, SHUTA HONDA, Nagoya University, HIROYOSHI ITOH, Kansai University, JUN-ICHIRO INOUE, Nagoya University, HIDEKAZU KUREBAYASHI, THEODOSSIS TRYPINIOTIS, C. H. W. BARNES, J. A. C. BLAND, University of Cambridge — We show that the IRSs (Interface Resonant States) within the Schottky barrier play an important role for the negative spin polarization of the current and its bias dependence, and compare with our experimental results [1]. We have calculated the spin polarization P of the tunnel conductivity using a full-orbital tight-binding model, and have shown that the IRSs within the Schottky barrier in the GaAs layer influence significantly the spin-dependent tunneling across the interface. It has been clearly shown that the band matching of the IRSs plays a crucial role on the spin polarization. The theoretical results account well for earlier experimental results including the tunneling of photo-excited electrons. The present results suggest that the spin polarization can be controlled by the Schottky barrier heights, and that a spin-switch device with bias control may also be promising. Quantitative performance of the device, however, needs more quantitative calculations including effects of atomic disorder for example. [1] H. Kurebayashi et al., Appl. Phys. Lett. 91, 102114 (2007).

10:36AM A22.00010 Time dependent analysis of spin transport in lateral semiconductor/ferromagnet structures with non-collinear magnetization, YANG SONG, Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627, HANAN DERY, Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York 14627 — We model the transport in lateral semiconductor channels beneath ferromagnetic contacts with non-collinear magnetization directions. We quantify the effects of the mixing conductance and of the spin polarization across the interface, of the electrical field in the channel and of the resistance ratio between the channel and the interface. We focus on a non-local spin valve geometry in which two contacts are biased and collinear and a third terminal is non-collinear and “semi” floating (connected in series with a capacitor). This structure can be used for memory devices with multi-valued stored bits by rotating the magnetization in one of the terminals and detecting the transient current signal that flows through the non-collinear terminal. The shape and magnitude of this current signal is strongly influenced by the relation between the non-collinear magnetization direction and the (2D) spin accumulation in the channel that is being set by the biased (collinear) contacts.

10:48AM A22.00011 Magnetic force detection of non-equilibrium electron spin-polarization in n-GaAs, VIDYA BHALLAMUDI, GANG XIONG, Dept of Physics, Ohio State University, Columbus, OH 43210, MARK BRENNER, Dept of Electric and Computer Engineering, Ohio State University, Columbus, OH 43210, YOUNGWOO JUNG, YURI OBUKHOV, DENIS PELEKHOV, Dept of Physics, Ohio State University, Columbus, OH 43210, STEVE RINGEL, Dept of Electric and Computer Engineering, Ohio State University, Columbus, OH 43210, P. CHRIS HAMMEL, Dept of Physics, Ohio State University, Columbus, OH 43210 — Magnetic Force Microscope (MFM) offers an alternative to optical and electrical techniques for detecting and imaging spin-polarized electron populations in semiconductor spintronic devices. Unlike other methods, MFM has the advantage of being material non-specific as it directly detects spins in the semiconductor through their magnetic dipole coupling to micromagnetic tip. However, it is challenging to achieve the high sensitivity required for sensing small non-equilibrium spin populations, orders of magnitude smaller than those in ferromagnetic materials. Here we present our progress developing a high sensitivity cryogenic MFM for imaging optically injected electronic spins in GaAs. Spins are created in an epitaxially grown In0.1Ga0.9As QW by optical injection from a nearby laser diode. The spin Hall effect induces a magnetic force due to the optically injected spins. Micro-magnetic tip generating large field gradient is used for enhancing the signal. We will show simulation results for the expected forces, taking spin relaxation, diffusion and local tip field into account. The status of spin imaging experiment will also be presented.

Monday, March 16, 2009 8:00AM - 10:48AM
Session A23 DCMP: Plasmons and Optical Absorption
8:00AM A23.00001 Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment, ARON WALSH, KWANG-SOON AHN, SUDHAKAR SHET, MUHAMMAD N. HUDA, TODD DEUTSCH, HELI WANG, JOHN A. TURNER, YANFA YAN, MOWAFAK M. AL-JASSIM, SU-HUIWEI, National Renewable Energy Laboratory — Discovery of a chemically stable, light absorbing and conductive metal oxide with band edges aligned to water redox potentials has been a goal of physical scientists for the past forty years. Despite an immense amount of effort, no solution has been uncovered. We will present the results of our combined theoretical and experimental exploration of a series of unconventional ternary cobalt spinel oxides, which offer chemical functionality through substitution on the tetrahedral spinel A site. First-principles predictions of the substitution of group 13 cations (Al, Ga, In) in Co$_x$O$_y$ to form a series of homologous CoO$_2$O$_x$ spinel compounds are combined with experimental synthesis and photoelectrochemical characterization. Ultimately, while tunable band gaps in the visible range can be obtained, the material performance is limited by poor carrier transport properties associated with small polarons. Future design pathways for metal oxide exploration will be briefly discussed.

8:12AM A23.00002 Multiple electron generation in a sea of electronic states, WAYNE WITZEL, Sandia National Laboratory, NM, ANDREW SHABAABE, George Mason University. ALEXANDER EFROS, CARL HELLBERG, JACOBS VERNE, Naval Research Laboratory — In traditional bulk semiconductor photovoltaics (PVs), each photon may excite a single electron-hole, wasting excess energy beyond the band-gap as heat. In nanocrystals, multiple excitons can be generated from a single photon, enhancing the PV current. Multiple electron generation (MEG) may result from Coulombic interactions of the confined electrons. Previous investigations have been based on incomplete or over-simplified electronic-state representations. We present results of quantum simulation that includes favorable conditions of configuration states and show how the quantum dynamics, even in a closed electronic system, yields a saturated MEG effect on a femtosecond timescale. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

8:24AM A23.00003 Quantum confined stark effect in non-identical InAs/GaAs coupled quantum dots: Dependence on vertical electrical field, MUHAMMAD USMAN, GERHARD KLIMECK, NCN Purdue University West Lafayette IN — InAs/GaAs coupled quantum dot (QDs) have gained much attention for optical and quantum computing applications. Due to strain, originating from assembly of lattice-mismatched semiconductors, quantum dot tend to grow in the vertical direction. These stacked QDs are strongly coupled through strain field, which is atomically inhomogeneous and penetrates deep into GaAs buffer layer surrounding the dots. Piezoelectric field must be taken into account to properly model the experimentally observed symmetry breaking and a global shift in the energy spectra of the system. Vertical electrical field applied in the growth direction results in the red shift of emission spectra due to the quantum confined stark effect. Previous studies are based on kp method that ignore the crystal symmetry, optical anisotropy and piezoelectricity effects. In this work, we apply a twenty band sp$^3$d$^*s$ atomic tight binding model to study the experimentally observed red shift of emission spectra resulting from an applied electrical field. We quantitatively compare the results for coupled QDs with the results for single QD.

8:36AM A23.00004 Experimental Kataura plot from individual Single-Wall Carbon nanotubes on silicon substrate, YA-PING HSIEH, MARIO HOFMANN, CHI-TE LIANG, MILDRED S. DRESSELHAUS, JING KONG, MIT — The dependence of Raman scattering of individual carbon nanotubes on excitation energy was investigated. For this carbon nanotubes were grown on Silicon substrate and their Raman spectra were analyzed for a multitude of different laser excitation wavelength. Resonance windows for several tubes within one family were measured to obtain the energy of maximum intensity of the Raman peak positions. By carefully calibrating these Raman peak positions, this experimental data can generate an experimental Kataura plot, which was compared to the theoretical prediction. Finally, a relation between RBM frequency and diameter was obtained based on the experimental Kataura plot. These results will improve the chirality assignment of carbon nanotubes grown on silicon substrate.

8:48AM A23.00005 Effect of Multi-Resonance Subband Structure on the Kerr Nonlinearity of Quantum-Cascade Lasers, JING BAI, University of Minnesota Duluth — This work focuses on the investigation of the optical Kerr lensing effect in quantum-cascade lasers with multiple resonance levels. The Kerr refractive index $n_2$ is obtained through the third-order susceptibility at the fundamental frequency $\chi^{(3)}(\omega)$. Resonant two-photon processes are found to have almost equal contributions to $\chi^{(3)}(\omega)$ as the single-photon processes, which result in the predicted enhancement of the positive $n_2$, and thus may enhance mode-locking of quantum-cascade lasers. Moreover, an isosceles optimization strategy for further improving $n_2$ through the band-structure design is also demonstrated, in order to boost the multimode performance of quantum-cascade lasers. Simulation results show that the optimized stepwise multiple-quantum-well structure has a twofold enhancement on $n_2$ over the original flat quantum-well structure. This leads to a refractive-index change $\Delta n$ of about 0.01, which is at the upper bound of those reported for typical Kerr medium. This stronger Kerr refractive index may be important for quantum-cascade lasers ultimately to demonstrate self-mode-locking.

9:00AM A23.00006 Anisotropic Electronic Screening due to Fermi Surface Nesting in Graphite, JAMES REED, University of Illinois, YOUNG IL JOE, DIEGO CASA, THOMAS GOG, Y. Q. CAI, PETER ABBAMONTE — We used inelastic X-ray scattering to measure the imaginary part of the density-density Green’s function, $\Im[\chi(\vec{k},\omega)]$, of a single crystal graphite sample along six directions in the basal plane from $[100]$ to $[110]$. To place $\Im[\chi(\vec{k},\omega)]$ on an absolute scale we calculate a scaling coefficient using the optical sum rule. The real part of $\chi(\vec{k},\omega)$ is calculated via the Kramers-Kronig transformation. We use an inversion algorithm to map the data into real space at various time intervals with attosecond time resolution. The images of the density response we produced show hexagonal anisotropy, which arises from scattering between the K and K’ points of the Brillouin zone. Analysis of the data at $\omega = 0$ provides us with the anisotropic induced electron density around a static impurity as function of distance. Integration of the local density around $\vec{r} = 0$ gives the effective charge of the impurity from which we deduced the background dielectric constant, $\varepsilon_{\infty}$, to be approximately 2.23.

1DOE grant: DE-FG02-07ER46459

9:12AM A23.00007 Plasmons in the presence of Tamm-Shockley states with Rashba splitting at noble metal surfaces, ABDEL-KHALEK FARID, EUGENE MISHCHENKO — Au(111) or similar noble metal surfaces feature Tamm-Shockley surface states that are known to possess considerable spin-orbit splitting of the Rashba type of order $\Delta = 0.1$ eV. When interacting with an electromagnetic field such states are expected to have resonances when the frequency of the field is near the energy of the spin-orbit splitting $\Delta$. They originate from the intersubband transitions between spin-split subbands and can be observed in the frequency dependence of the surface impedance. Plasmons in thin metal films are gapless and can be strongly affected by these spin resonances, acquiring significant modification of the spectrum when it intersects the $\omega = \Delta$ line. Finally, an interesting demonstration of the intersubband resonances can be achieved when metal films are coated with ionic dielectrics that have a frequency of longitudinal/transverse optical phonons above/below $\Delta$. The dielectric function between the two optical phonon frequencies is negative which forbids propagation of conventional plasmon-polaritons. However, the presence of spin-orbit-split surface states allows plasmon-polaritons to exist in this otherwise forbidden range of frequencies.

1This work was supported by DOE, Award No. DE-FG02-06ER46313.
9:24AM A23.00008 Phases Shift in Sub-wavelength Plasmonic Hole on Thin Metal Film. JUN XU, HYUNJIN MA, NICHOLAS X. FANG, University of Illinois at Urbana-Champaign — While recent study of extraordinary transmission of light through sub-wavelength plasmonic nanostructures shows promise of novel nanophotonic elements in sensing and display, the origin of such phenomena is still under hot debate. In this paper, we measured the phase delay of the squeezed light emerging from individual plasmonic holes. Near-field Scanning Optical Microscope (NSOM) has been used to measure the interference of transmitted and scattered light of an isolated sub-wavelength hole on thin metal film. Our results indicate that even with a 30nm perforated film, the observed phase shift can be as large as 300 degrees, well beyond the prediction from earlier theoretical models. Counter intuitively, the measured phase shift is sensitive to the wavelength, the film thickness but insensitive to hole diameter. Also, full scale simulation by COMSOL has been done to show the more detail features inside the metal film. Our study may provide new insight to compact and efficient optoelectronic devices.

1This project is supported from DARPA, ONR and NSF.

9:36AM A23.00009 Coupling between Surface Plasmon Resonance and electric current in Au stripes, MIGUEL ANGEL GARCIA, AIDA SERRANO, JOSE DE LA VENTA, Dpt. Material Science. University Complutense at Madrid, Spain. — Surface Plasmon Resonance (SPR) is the most outstanding feature of noble metal films. SPR consists on a collective oscillation of the conduction electrons when excited optically in the appropriate geometrical and energy conditions. The electrical current passing trough the metal film involves also the movement of conduction electrons. Thus, coupling effects are expected between SPR and electrical resistivity. A modification of the SPR when a electrical current passes through the film, could allow the modulation of an optical signal by a electrical one. Similarly, when the film is illuminated at the SPR conditions, the oscillation of the conduction electrons and local heating can induce an enhancement of the electric resistivity that can be used to translate an optical signal into a electric one. Those effects could be useful in the development of new fast optoelectronic transducers. We present here results on Au stripes illuminated to induce the SPR while electric currents flow with different orientation with respect to the light polarization.

9:48AM A23.00010 Surface plasmon resonance enhanced binding of metal nanoparticles, K.L. CHAN, M.J. ZHENG, K.W. YU, The Chinese University of Hong Kong. — The interparticle force between metallic nanoparticles illuminated by laser light has been studied theoretically. When the distances between the particles are sufficiently small, the excitation of surface plasmon modes within these particles can lead to strongly enhanced laser fields. As a result, there are strongly enhanced light-induced binding forces between these nanoparticles. For physically realizable laser power, these forces can exceed the van der Waals forces by several orders of magnitude. In our theoretical calculations, we considered the interparticle force and potential between two approaching metal nanoparticles. The metal particles are routinely modelled as Drude metallic spheres, and the interparticle force has been captured conveniently by an approximate multiple image formula between two spheres. When the incident light frequency is near the surface plasmon resonance frequency, we find that the force varies nonmonotonically with the distance and a stable local minimum in the potential energy can be found, signifying a binding between the particles. On the experimental and technological side, these studies are also crucial to optical spectroscopy in the nanoscales. Work supported by the General Research Fund of the Hong Kong SAR Government. [1] J. P. Huang, K. W. Yu, G. Q. Gu Electrorotation of a pair of spherical particles, Phys. Rev. E, Vol. 65, art. no. 021401 (2002).

10:00AM A23.00011 Giant Electric Field Generation in Nano-Metallic Cylinder Chains Due to Plasmon Propagation, ANGELA CAMACHO, JUAN CARLOS ARIAS, Universidad de los Andes — We present a study of the superficial plasmons propagation in a chain of nano-metallic cylinders by analyzing: size effect and coupling between the particles. Particularly, we focus on the main features of electric fields in the inter-cylinder regions due to their relationship with SERS(Surface-enhanced Raman Scattering). Giant electric fields have been observed in spherical nano-particles showing an enormous increasing of the cross section, which offers very interesting applications in molecular physics. We calculate the external radiation effect on chains of cylinders lateral and vertically coupled and examine the Plasmon formation in them. Specially, we study the Plasmon propagation depending on the particle size, the separation between them and the type of coupling. We find enhanced electric fields in the inter-particles regions showing the charge accumulation and order effects in cylinders, which are strongly dependent on the two above proposed parameters, and we also extend our results to possible Surface Enhanced Raman Scattering geometric effect to make a comparison with the spherical nano-particles.

10:12AM A23.00012 Optical properties of medium size noble and transition metal nanoparticles, JUAN C. IDROBO, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory. — Using first-principles methods within time dependent density functional theory and the local density approximation (TDLDA) the absorption spectra of medium size (~20-80 atoms) silver, gold and copper nanoparticles have been calculated. The nanoparticles are fcc fragments with different aspect ratios. We find that in the case of Ag nanoparticles is well reproduced by classical electrodynamics theory based in Mie’s formalism, using the dielectric function of bulk Ag and taking into account the nanoparticle shape. For the case of Cu and Au, there is a similarity in the overall features of the quantum mechanical and classical spectra, but no detailed agreement. We will discuss the role that the d-electrons among all the different elements and the surface states play in controlling the optical properties of the nanoparticles. This work was supported by GOALI NSF grant (DMR-0513046), DOE, the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, and Alcoa Inc.

10:24AM A23.00013 Electronic Coupling and Optimal Gap Size within a Metal Nanoparticle Dimer, KE ZHAO, CLAUDIA TROPAREVSKY, University of Tennessee and Oak Ridge National Laboratory, DI XIAO, Oak Ridge National Laboratory, ADOLFO EGUILUZ, University of Tennessee and Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory and University of Tennessee. — We study the electronic coupling between two metal nanoparticles using density functional theory methods. We show that a continuous change in the particle separation leads to an abrupt transition from strong to weak electronic coupling, which defines an optimal separation for the dimer. While in the weak-coupling regime the dimer behaves like isolated clusters, its crossing into the strong-coupling regime is signified by two distinct phenomena, namely, the onset of a net magnetic moment, and a maximum in the static polarizability. We also show that as the system switches over from strong to weak coupling regime, the response to an applied electric field is nonlinear even for very small fields. The strong dependence of the coupling on the atomic structure of the nanoparticles and their orientation is also discussed. Our study is expected to have an impact on a variety of systems composed of aggregates of nanoparticles.

1Work supported by DMSE/BES of DOE, NSF and PCSCS/CMSN programs.
10:36AM A23.00014 Extraordinary Optical Transmission through Circular Nanotrenches in Ag Films , FENG WANG, Liquid Crystal Institute, Kent State Univ., MIN XIAO, Department of Physics, University of Arkansas, QIHOU WEI, Liquid Crystal Institute, Kent State Univ., LIQUID CRYSTAL INSTITUTE, KENT STATE UNIV. TEAM, DEPARTMENT OF PHYSICS, UNIVERSITY OF ARKANSAS COLLABORATION — This work reports studies on the extraordinary transmission of normally incident light through sub-wavelength circular nanotrenches in Ag films. The concentric periodic nanotrenches are perforated through 100nm thick Ag films by using focused-ion beam (FIB). Far-field transmission measurements show that under the illumination of linearly polarized white light, the transmitted light is not linearly polarized and exhibits broad-band enhanced transmission with the center wavelength varying with the periodicity of the trench. These spectroscopic experimental results can be reproduced qualitatively through finite-difference time domain (FDTD) simulations. Especially, simulations show that the transmitted light is radially polarized at low frequencies, while azimuthally polarized at high frequencies. These interesting polarization statuses can be explained as a result of competition between transmission of s and p polarized light through periodic gratings of nanotrenches.

Monday, March 16, 2009 8:00AM - 10:48AM –
Session A24 DMP: Focus Session: Nanotube Synthesis 326

8:00AM A24.00001 Thermodynamic instabilities in nano-catalysts and their effects on the diameter of grown nanotubes1, STEFANO CURTAROLO, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, Durham NC 27708 — Fe and Fe-Mo nanoclusters are becoming the standard catalysts for growing single-walled carbon nanotubes (SWCNTs) via chemical vapor decomposition (CVD). Contrary to the Gibbs-Thomson formalism, experimental results show that reducing the size of the catalyst beyond a certain limit requires increasing the (minimum) growth temperature. This apparent paradox is addressed in terms of solubility of C in Fe nanoclusters. By using first principles calculations, an innovative thermodynamic model is constructed to determine the behavior of the phases competing for stability. As a function of particle size, there are three scenarios: steady state-, limited-, or no-growth of SWCNTs, corresponding to unaffected, reduced, and zero solubility of C in the clusters. The results are extended to Fe-Mo binary catalysts. The 15+ year-long-standing question about the effects of Mo concentration on the growth capability is finally answered. Phys. Rev. Lett. 100, 195502 (2008), Phys. Rev. B, 77, 115450 (2008), Phys. Rev. B 75, 205426 (2007).

1Research sponsored by ACS and Honda R.I.

8:36AM A24.00002 CVD grown SWCNTs on Si substrate from DPN patterned catalyst precursor, IRMA KULJANISHVILI, RACHEL KOLTUN, SCOTT MAYLE, VENKAT CHANDRASEKHAR, Department of Physics & Astronomy, Northwestern University, DMITRIY DIKIN, Department of Mechanical Engineering, Northwestern University, SERGEY ROZHOK, Nanofink, Inc. — Much interest has been generated around patterning and synthesis of high quality single wall carbon nanotubes (SWCNTs) into desired architectures. Here we report our work, undertaken to elucidate a simple method for delivering catalyst nanoparticles on defined locations on Si substrate via direct writing approach. We applied the Dip-Pen Nanolithography (DPN) approach to pattern catalyst nanoparticles in selective locations on the substrate, and using this technique, we developed a successful recipe for the subsequent CVD growth to produce high quality SWCNTs into scalable array geometries. Key parameters for successful implementation of this technology into devices or circuit architectures will be discussed. We will present our results on patterning, synthesis and characterization of SWCNTs as grown on the substrate. Raman spectroscopy analysis, electrical and thermal properties of individual SWCNTs prepared into complex nanodevices will be presented in progress.

1Support by DOD, Army Reserach Office.

8:48AM A24.00003 Effective Growth of Boron Nitride Nanotubes by Thermal-CVD1, CHEE HUEI LEE, MING XIE, DEREK MEYERS, JIESHENG WANG, YOKE KHIN YAP, Department of Physics, Michigan Technological University, 1400 Townsend Dr, Houghton, MI 49931 — The synthesis of boron nitride nanotubes (BNNTs) are challenging as compared to the growth of carbon nanotubes (CNTs). Most of reported techniques required unique setup and temperatures >1300 °C. Here we show that clean and long multiwalled BNNTs can be grown by simple catalytic thermal CVD. This was obtained by a growth vapor trapping approach inspired by the whisker nucleation theory. Based on our new findings, we have achieved patterned growth of BNNTs at desired locations. High resolution TEM shows that these BNNTs are highly crystallized. Besides, the tangential vibrational mode predicted by theory was detected in our BNNTs. This vibration mode could be the fingerprint for BNNTs with high crystallinity.

1YKYP acknowledges support from the NSF CAREER award (DMR#0447555) and DOE BES (DE-FG02-06ER46294).

9:00AM A24.00004 Co-optimizing carbon nanotube synthesis: control of diameter, structural quality, and growth kinetics along with simultaneous cost minimization , ERIC R. MESHOT, Department of Mechanical Engineering, University of Michigan, DESIRÉE L. PLATA, Department of Civil and Environmental Engineering, MIT, Marine Chemistry and Geochemistry Department, Woods Hole Oceanographic Institute, CHRISTOPHER M. REDDY, Marine Chemistry and Geochemistry Department, Woods Hole Oceanographic Institute, PHILIP M. GSCHWEND, Department of Civil and Environmental Engineering, MIT, A. JOHN HART, Department of Mechanical Engineering, University of Michigan — We employ a decoupled CVD method that not only facilitates control of mean diameter and structural quality of vertically aligned CNTs, but also co-optimization of kinetics for efficient growth to “forest” heights of several millimeters. The growth substrate temperature (Ts) governs agglomeration of the catalyst film which primarily determines CNT diameter, while structural quality monotonically increases with Ts. Independent heating (Tp) of the reactant mixture generates a strikingly diverse population of active hydrocarbons. These analyses, in concert with real-time laser measurements of forest growth rate and height suggest that select products of gas treatment promote growth, while excessive gas-phase pyrolysis of hydrocarbons adversely affects the CNT structure. Further, we directly inject select compounds in the absence of thermal treatment, thus minimizing energetic costs.

9:12AM A24.00005 Diameter and Geometry Control of Vertically Aligned SWNTs through Catalyst Manipulation , RONG XIANG, ERIK EINARSSON, JUN OKAWA, YOICHI MURAKAMI, SHIGEO MARUYAMA, Department of Mechanical Engineering, The University of Tokyo — We present our recent progress in manipulating our liquid-based catalyst loading process, which possesses greater potential than conventional deposition in terms of cost and scalability, to control the diameter and morphology of single-walled carbon nanotubes (SWNTs). We demonstrate that the diameter of aligned SWNTs synthesized by alcohol catalytic CVD can be tailored over a wide range by modifying the catalyst recipe. SWNT arrays with an average diameter as small as 1.2 nm were obtained by this method. Additionally, owing to the alignment of the array, the continuous change of the SWNT diameter during a single CVD process can be clearly observed and quantitatively characterized. We have also developed a versatile wet chemistry method to localize the growth of SWNTs to desired regions via surface modification. By functionalizing the silicon surface using a classic self-assembled monolayer, the catalyst can be selectively dip-coated onto hydrophilic areas of the substrate. This technique was successful in producing both random and aligned SWNTs with various patterns. The precise control of the diameter and morphology of SWNTs, achieved by simple and scalable liquid-based surface chemistry, could greatly facilitate the application of SWNTs as the building blocks of future nano-devices.
9:24AM A24.00006 Ethanol-promoted growth of dense vertically aligned small-diameter carbon nanotubes. Yong-Yi Zhang, University of Michigan, John Gregoire, Cornell University, John Hart, University of Michigan — We report the use of a small concentration of ethanol in addition to ethylene as the carbon source for growth of vertically aligned CNT "forests." In our system, adding ethanol promotes the catalyst lifetime from approximately 20 minutes to nearly 60 minutes, and accordingly increases the forest height from 2.5 mm to over 5 mm, with CNT diameters of approximately 5 nm (2-3 walls). Spread composition films deposited by gradient sputtering, combined with non-destructive mapping of CNT diameter and alignment by small-angle X-ray scattering, enable high-throughput discovery of necessary and sufficient conditions for growth of small-diameter CNTs. Compared with the widely known water-assisted "super growth" process, we find that ethanol enables much finer control of the dewpoint and thus offers more consistent and tunable results. Also, ethanol is a weaker oxidant than water and therefore creates fewer structural defects due to unwanted etching of the CNT walls.

9:36AM A24.00007 Manufacturing thin films of densely packed horizontally aligned carbon nanotubes. Sameh Tawfick, A. John Hart, University of Michigan — Dense packing of carbon nanotubes (CNTs) over long-range dimensions is necessary to replicate their outstanding properties in functional thin films. We present a continuous method for transforming pillars of vertically aligned (VA) CNTs into densely packed, horizontally aligned (HA) CNT ribbons and sheets, which can be directly used on wafer-scale dimensions and/or patterned by photolithography and plasma etching to achieve feature dimensions down to the micron scale. In this process, a small roller is used to "topple" millimeter-tall VA-CNT microstructures and to simultaneously compress them, thus increasing the packing fraction of CNTs from 2% to 60%. We formulate design guidelines for selection of pattern geometry, roller diameter and material, and the kinetics of the rolling motion. This enables precise control of the HA-CNT film topography and thickness, and the packing density and orientation of the CNTs. Nanoindentation of the HA-CNT films reveals that the initial tortuosity of the VA-CNT forest determines the ultimate achievable densification. Electrical conductivity of ribbons is characterized using dc-four-point testing of lithographically-patterned CNT ribbons with Au contacts. The HA-CNT structures are easily transferred to other substrates, enabling integration with CMOS and MEMS fabrication, and with alternative substrates such as flexible plastics.

9:48AM A24.00008 Incremental Growth of Single-Wall Carbon Nanotube Arrays Explored by Pulsed CVD. Jeremy Jackson, Oak Ridge National Laboratory, Alex Puretzky, Igor Merkulov, Christopher Rouleau, Karrenmore, Norbert Thonnard, Cyula Eres, David Geohagen, CNMS and MSTD Divisions, Oak Ridge National Laboratory Team — Gas pulses of variable duration and peak flux were used to explore the incremental growth and evolution of alignment of vertically-aligned carbon nanotubes arrays (VANTA)s by typical chemical vapor deposition within a tubular reactor. Time-resolved reflectivity from Fe/Al catalyst-coated Si substrates was used to follow the growth of the arrays after the arrival of successive acetylene gas pulses injected into fast argon-hydrogen flows at 6 Torr total pressure. The evolution of alignment of the arrays measured with the in situ optical reflectivity data was correlated with SEM images for growth resulting from single- and multiple-pulse growth. The incremental length per pulse was varied from 20 nm to several microns in less than a second, corresponding to growth rates ranging up to 7 microns/second. Effects of repeated reぬcleation of growth along the nanotube wall structure were measured by HRTEM and Raman spectroscopy.


10:00AM A24.00009 A model of dry-drawing of multiwall carbon nanotube forest into self-assembled sheets and yarns. Alexander Kuznetsov, Alexandre Fonseca, Ray Baughman, Anvar Zakhidov, NanoTech Institute, University of Texas at Dallas — A dry-state technique to produce highly-oriented, free-standing multiwalled carbon nanotube (MWNT) sheets and yarns which are mechanically strong, transparent, and highly oriented has been developed recently [1,2]. A model which allows to describe the main features of the process of dry-drawing self-assembly of vertically oriented multiwall carbon nanotube (MWCNT) forest into horizontal MWCNT sheets or yarns is developed in this presentation. The model is based on two main concepts: 1. self-strengthening of nanotube bundle interconnects during the bending-pulling process; 2. rearrangement of bundles by accordion-type stretching motion accompanied by detachment of bundles (at the top and bottom of the forest). This detachment occurs due to unzipping and self-strengthening of interconnects beyond a critical force, which permits to pull the next bundle from the forest, keeping the process of dry-drawing continuous. Developed model determines the parameters of CNT forest for which the dry-drawing is possible. It also allows to estimate such properties of the produced sheets and yarns as length, density, strength and electrical conductivity. [1] M. Zhang et al., Science 2005, 309, 1215. [2] M. Zhang et al., Science 2004, 306, 1358.

10:12AM A24.00010 Termination mechanism of carbon nanotube forest growth. Mostafa Beidelberg, Eric R. Meshot, Yongyi Zhang, Haicheng Guo, University of Michigan, Erica Verploegen, Massachusetts Institute of Technology, Wei Lu, A. John Hart, University of Michigan — Understanding the termination event in the growth of carbon nanotubes (CNTs) by chemical vapor deposition (CVD) is a roadblock in the pursuit of ultra-long CNTs, which would be useful for many of applications. We present in situ measurements show that vertically-aligned CNT "forest" growth terminates abruptly, which is not predicted by widely suggested models of diffusion-limited growth. In this work, we complement forest height measurements with mass and density measurements, and with spatial mapping of CNT diameter, alignment, and spacing along the forest sidewall by small-angle and ultra-small-angle synchrotron X-ray scattering (SAXS, USAXS). Accordingly, we reveal that the areal density of growing CNTs begins to decay long before the forest height terminates, indicating that gradual deactivation of catalyst particles is collectively responsible for the limitation to CNT forest height. Considering that mechanical and surface interactions among CNTs create the self-supporting forest structure, a gradual decay of CNT density can lead to an abrupt loss of CNT alignment at the forest base when the CNT-CNT spacing increases sufficiently. This proposed mechanism is supported by finite element models of CNT-CNT buckling and contact.

10:24AM A24.00011 Clarifying the Rules for the Highly Efficient Growth of Carbon Nanotubes. Don Futaba, Jundai Gotou, Satoshi Yasuda, Takeo Yamada, Motoo Yumura, Kenji Hata, Nanotube Research Center, AIST — In water-assisted chemical vapor deposition (CVD), the addition of a growth enhancer, e.g. water, to the ambient of normal hydrocarbon dramatically improves growth efficiency resulting in vertically aligned forests [1]. Here, we present a generalized picture of water-assisted CVD (Super-growth) by demonstrating that highly efficient growth of carbon nanotubes (CNTs) is possible by, essentially, a countless number of growth enhancers exemplified here by alcohols ethers, esters, ketones, aldehydes, and even carbon dioxide. From an extensive investigation, we found that the key for highly efficient growth is to use two essential ingredients: 1) a carbon source not containing oxygen, and 2) a growth enhancer containing oxygen. We believe that this new understanding of CNT synthesis further cultivates and expands the world of CVD where innumerable new and completely unexplored growth ambitions can emerge that would lead to further scientific discovery [1] K. Hata et al, Science, 306, 1241 (2004).

10:36AM A24.00012 ABSTRACT WITHDRAWN —

Monday, March 16, 2009 8:00AM - 11:00AM —
Session A25 DMP: Focus Session: Graphene I: Electronic Properties
Due to Klein's tunneling, the relativistic electron in graphene cannot be localized by a confinement potential. In this case electron states in a graphene quantum dot become resonances with finite trapping time. We consider these resonances as the states with complex energy. To find the energies of these states we solve the time-independent Schrodinger equation with outgoing boundary conditions. The imaginary part of the energy determines the width of the resonances and the electron trapping time. We show that if the parameters of the confinement potential satisfy a special condition, then an electron can be strongly localized by such quantum dot, i.e., the trapping time becomes infinitely large. We show how a deviation from this condition affects the electron trapping time. We also analyze the energy spectra of an electron in a graphene quantum ring with a sharp boundary. We show that in this case the condition of strong trapping can be tuned by varying parameters of confinement potential, e.g., internal radius of the ring.
10:12AM A25.00010 Thermally assisted self-trimming of graphene nanoribbon edges. YANG, DAVID TOMÁNEK, Michigan State University; SAVAS BERBER, Gebze Institute of Technology — Edge morphology is known to play a key role in the conductance of graphene ribbons. We use a combination of ab initio density functional total energy and molecular dynamics calculations to investigate thermally induced reconstruction occurring at graphene edges. The calculated total energy surfaces suggest that along all nanoribbon sites, atoms at edge defect sites require least energy to be displaced. At elevated temperatures, these atoms will primarily participate in diffusion and related processes at the edge that will gradually reduce the edge roughness and thus lower the edge energy. We explore various scenarios leading to such self-trimming of edges, including concerted migration processes and unravelling of chains at the edge. Close inspection of our results suggests that the preferential mechanisms and activation barriers for trimming of rough armchair and zigzag edges may be different. In selected scenarios, Joule heating of nanoribbons may not only straighten rough edges, but also modify the preferred edge morphology.

1Supported by NSF NIRT grant ECS-0506309 and NSF NSEC grant EEC-425826.

10:24AM A25.00011 Fermi surface of graphene on Ru(0001). THOMAS BRUGGER, HUGO DIL, JÜRGEN OSTERWALDER, THOMAS GREBER, Physik-Institut, Universitaet Zuerich, Winterthurerstrasse 190, CH-8057 Zuerich, Switzerland; BERNHARD BOCQUET, Universite de Lyon, Laboratoire de Chimie, Ecole Normale Superieure de Lyon, CNRS, France, SEBASTIAN GÜNTHER, JOOST WINTTERLIN, Department Chemie, Ludwig-Maximilian Universitaet, Butenandstrasse 5-13, D-81377 Muenchen, Germany — The structure of a single layer graphene on Ru(0001) is compared with that of a single layer hexagonal boron nitride nanomesh on Ru(0001). Both are corrugated sp² hybridized networks and display a π-band gap at the K point of their 1×1 Brillouin zone. In contrast to h-BN/Ru(0001), g/Ru(0001) has a distinct Fermi surface which indicates that 0.1 electrons per 1×1 unit cell are transferred from the Ru substrate to the graphene. Photoemission from adsorbed xenon on g/Ru(0001) identifies two distinct Xe 5p1/2 lines, separated by 240 meV, which reveals a corrugated electrostatic potential energy surface like on h-BN/Rh(111) [1]. These two Xe species are related to the topography of the template and have different adsorption energies.


10:36AM A25.00012 Complex refractive index of graphene measured by picometrology. XUEFENG WANG, DAVID NOLTE, Purdue University — The complex refractive index ñg of graphene remains unresolved because the traditional technique, ellipsometry, fails when applied to graphene with its sub-nanometer thickness, dielectric anisotropy, and small transverse sample size. Here we apply interferometric picometrology to measure ñg at 488 nm, 532 nm and 633 nm. A strong dispersion of ñg was found in the visible region. ñg varies from 2.4-1.0i at 532 nm to 3.0-1.4i at 633 nm at room temperature. The dispersion is five times stronger than bulk graphite (2.67-1.34i to 2.73-1.42i from 532 nm to 633 nm). In experiments, Graphene is deposited on a substrate with complex reflection coefficient r̃ tuned near an antinode condition. As a dielectric film, graphene modifies r̃ of the substrate into r̃′. Picometrology measures both the amplitude and the phase change of r̃′, and therefore acquires the full information needed to calculate ñg. This is accomplished by scanning a normal-incidence focused Gaussian beam (1.5 μm width) over the graphene and monitoring the asymmetric diffraction of the reflected beam. Picometrology measures the complex change of r̃ with a quadrant detector that simultaneously monitors both intensity and axis shift of the reflected beam and calculates ñg. The strong dispersion of graphene is reported here for the first time, and it is likely caused by the strongly modified quantum level structure of the single atomic layer.

10:48AM A25.00013 Zero-bias conductance anomaly in point-contact junctions on graphite. WANG, KYU PARK, CESAR CHIALVO, RICH JONES, SAM JOHNSON, NADYA MASON, LAURA GREENE, University of Illinois at Urbana-Champaign — The electronic properties of graphite, a two-dimensional carbon allotrope, continue to attract great interest because of the interesting underlying physics and application potential of this novel electronic material. An ideal single-layer graphene is known to show a linear behavior in the electronic density of states (DOS) around the Fermi level. The ability to engineer the DOS of single- and multi-layer graphene is considered as a fundamental requirement for the realization of electronic devices. To investigate the electronic DOS in graphene/graphite, we adopt a spectroscopic technique based on nanoscale point-contact junctions, where differential conductance spectra are taken at around the liquid helium temperature. A common feature observed in all junctions on both Kish graphite and HOPG is an anomalous conductance dip at zero bias. The conductance curves show a logarithmic bias dependence in their slopes, exhibiting a systematic evolution as a function of magnetic field and contact pressure. We discuss possible origins of these behaviors including the possibility of modification in the electronic DOS of graphite.

1Work supported by the U.S. DOE under Award No. DE-FG02-07ER46453.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A26 DMP DCOMP: Focus Session: Computational Nanoscience I: Inorganic Nanostructures and Interfaces 328

8:00AM A26.00001 Interface electrostatics in ferroelectric capacitors from first principles. MASSIMILIANO STENGEL, UCSB — Capacitors based on ferroelectric perovskites are potentially attractive for applications in nanoelectronics, such as non-volatile random-access memories and high-permittivity gate dielectrics. Thin-film geometries are sought after for optimal efficiency and information storage density. However, in such a regime, strong size effects arise that generally deteriorate the overall performance of the device. Understanding the properties of the oxide/electrode interface is crucial to overcoming these deleterious effects. In this talk I will present our recently-developed methodologies for working at fixed electric displacement field in first-principles density-functional calculations. I will show that application of fixed-D methods to ferroelectric capacitors provides enhanced flexibility for the study of interface-specific issues. I will demonstrate this technique by presenting results for a range of systems based on PbTiO₃ electric displacement field in first-principles density-functional calculations. I will show that application of fixed-oxide/electrode interface is crucial to overcoming these deleterious effects. In this talk I will present our recently-developed methodologies for working at fixed electric field.

8:36AM A26.00002 Multiexciton absorption in CdSe nanocrystals. ALBERTO FRANCESCHETTI, YONG ZHANG, National Renewable Energy Laboratory — Efficient multiple-exciton generation (MEG) has been recently reported in semiconductor nanocrystals. In this process, a single absorbed photon generates two or more electron-hole pairs. The MEG efficiency has so far been evaluated assuming that the change (bleaching) of the absorption spectrum due to MEG is linearly proportional to the number of excitons (Nₓ) that are present in the nanocrystal. We have examined this assumption using atomistic pseudopotential calculations for colloidal CdSe nanocrystals ranging in size from 3 to 4.6 nm. We found that the bleaching of the first absorption peak, ∆X₁, depends non-linearly on Nₓ, due to carrier-carrier interactions. When a single exciton is present in the nanocrystal, the 1s exciton peak is already 65-75% bleached. This non-linearity mandates an upper bound of 1.5 to the value of the normalized bleaching that can be attributed to MEG, significantly smaller than the limit of 2.0 predicted by the linear scaling assumption. Thus, measured values of the normalized bleaching in excess of 1.5 in CdSe nanocrystals cannot be due entirely to MEG, but must originate in part from other mechanisms.

1Funded by DOE-SC-BES-MSED, through NREL contract DE-AC36-08GO28308.
8:48AM A26.00003 Electronic Structure of Thiolate Covered Gold Nanoparticles1. YAN LI, GIULIA GALLI, FRANCOIS GYGI, University of California, Davis — We present ab initio calculations of the structural, electronic, and bonding properties of thiolate-covered gold nanoparticles that have been crystallized in recent experiments (Au$_{1102}$ (MBA)$_{14}$)[1]. We simulated exactly the same system as investigated experimentally (1596 atoms) and the results of our structural optimization confirm the stability of the experimentally determined structure. We find that the crystallized solid is a semiconductor with a sizable energy gap (~0.5 eV; within DFT), and electronic states at the valence band maximum and conduction band minimum are extended over the gold nanoparticle core and the interface. This energy gap appears to be insensitive to the type of adsorbate. We find a tendency of different adsorbate to exert “pull-out” forces on the surface gold atoms, and our analysis of chemical bonding supports the hypothesis that gold s electrons are donated to the MBA radicals so as to form a highly stable 58-electron, filled electronic shell structure. Finally, comparisons between adsorption energies in the case of gold nanoparticle and flat surfaces show that a finite curvature of the interface enhances the stability of Au-S bonds.

9:00AM A26.00004 Covalently Bonded Aromatic Molecules on Gold using a GW Approach1. ISAAC TAMBLYN, Dalhousie University, SU YING QUEK, Molecular Foundry, LBNL, STANIMIR A. BONEV, Dalhousie University, JEFFREY B. NEATON, Molecular Foundry, LBNL — Frontier molecular orbital energies dictate the nature of optical absorption, chemical reactivity, and charge injection at metal-organic interfaces. Recent work [1] on the conductance of benzenediamine-Au single-molecule junctions has shown that standard methods based on density functional theory fail to correctly position molecular orbitals relative to the Au Fermi level, resulting in a pathological overestimate of the conductance for this class of systems. In this work, we use many-electron perturbation theory within the GW approximation to compute quasiparticle energies of aromatic molecules covalently bonded to a gold surface, taking particular care to assess dynamical screening beyond standard plasmon-pole approximations. We discuss results for benzene on Au(111) bound via amine (-NH$_2$) and thiol (-SH) link groups. These data are compared with more approximate model self-energy corrections applied to these systems [1], and also recent experiments. [1] Quek et al, Nano Lett. 7, 3477 (2007).

9:12AM A26.00005 First-principles studies of interfacial charge separation in nano-materials photovoltaic heterojunction1. YOSUKE KANAI, University of California, Berkeley — Charge separation is a crucial process that must be understood in order to make substantial improvements in nano-materials based PV cells. In our work, first principles quantum mechanical calculations are employed to shed light on this process for some important nano-material heterojunctions. I will first present our work on the interfacial charge separation in Fullerene/P3HT and CNT/P3HT heterojunctions. Our findings indicate that in the fullerene system a two-step process is operative, involving an adiabatic electron transfer and an exciton dissociation via quasi-degenerate states localized on the fullerene. For the nanotubes, on the other hand, while such a two-step process is not necessary for efficient charge separation, the presence of metallic nanotubes lead to undesirable charge traps. Secondly, I will discuss how we are addressing the difficulty in employing standard DFT approaches for investigating inorganic-organic PV interfaces, which are composed of two distinct materials with very different electronic environments. I will discuss a QMC scheme for obtaining many-body corrections to the Kohn-Sham level alignments and its application to a CdSe/Oligothiophene hybrid PV interface, with the aim of tailoring its behavior by controlling the conjugation length.

9:48AM A26.00006 Nanoscale phase stability reversals in titanium oxide polymorphs. PAUL KENT, Oak Ridge National Laboratory, DANIËL HUMMER, JAMES KUBICKI, Pennsylvania State University, JEFFREY POST, Smithsonian Institution, PETER HEANEY, Pennsylvania State University — A surprising discovery of nanoscience is the reversal in relative stability of materials with the same composition but different structures as particles evolve from the nanoscale to the macroscopic. These reversals can be problematic, as they frequently induce the precipitation of metastable contaminant phases during the synthesis of compounds of interest. To investigate the fundamental origins of this phenomenon, we have (1) performed a series of large scale density functional calculations to characterize the energetics of the stability reversal between rutile and anatase nanoparticles, and (2) experimentally monitored the hydrothermal crystallization of titania nanoparticles using in-situ x-ray diffraction. Although the phenomenon of stability reversal is commonly explained as a domination of the crystalline surface energy as a fraction of the total energy, we find computationally that the refined average surface structures cannot account for the stabilization of nano-anatase relative to nano-rutile, even for 3nm sized particles. Instead we find that defects associated with the edges and corners of nanocrystals contribute significantly to the energy and must be included in any description of the stability reversal.

10:00AM A26.00007 Domain boundary formation in helical multishell gold nanowire, TAKEO HOSHII, Tottori University, TAKEO FUJIWARA, University of Tokyo — Helical multishell gold nanowire (Y. Kondo and K. Takayanagi, Science 289, 606 (2000)) is studied by molecular dynamics simulation with electronic structure (“ELSES” http://www.elses.jp/), so as to explore formation mechanism of helical domain boundary. We have proposed a model for the formation of helical multishell gold nanowires with molecular dynamics simulation with electronic structure (Y. Iguchi, T. Hoshi, T. Fujiiwara PRL 99, 125507 (2007)). In this paper, we show simulation results with larger samples, of which the rod length is more than 10 nm and the number of rod atoms is more than one thousand. Unlike the results of shorter rods in the previous paper, a well-defined domain boundary between helical and (non-)helical regions appears, when an atom moves from a inner shell into rod surface. The inserted atoms on the rod surface causes a surface reconstruction on rod surface and introduces a helical region with a domain boundary. Such an inserted atom is a possible candidate of mechanism for forming a helical rod from an ideal (non-helical) one.

10:12AM A26.00008 Plasmon resonance of gold nanoparticles: the effect of surfactants and solvents1. JEREMY NEAL, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — Metallic nanoparticles dispersed in host materials have many potential applications due to their unique optical properties. These properties are determined not only by the size, shape and composition of the particles, but also by their environment. Metallic nanoparticles are typically coated with surfactants to prevent aggregation; these surfactants can also significantly affect their optical response. The role of surfactant coatings has been studied previously, but the results are incomplete. We have obtained theoretical expressions to describe and have carried out numerical simulations to determine the effects of solvents and surfactants on the optical response.

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.
10:24AM A26.00009 Investigation of atomic oxygen embedment into copper surface by DFT calculation. MINYOUNG LEE, ALAN MCGAUCHY, Carnegie Mellon University, SUSAN SINNOTT, SIMON PHILLPOT, University of Florida, JUDITH YANG, University of Pittsburgh — In the oxidation of a Cu(100) surface, the Cu$_2$O islands grow both into the substrate and parallel to the surface. To investigate the oxide growth into the copper surface, we analyzed oxygen embedment using DFT calculations. Using the nudged elastic band method, we calculated energy barriers for oxygen embedment for different oxygen coverages and different surface morphologies. As the oxygen coverage increases from 0.25 monolayers (ML) to 1.0 ML, the energy barrier decreases and we find an energetically favorable site between the top and second copper layers at an oxygen coverage of 1.0 ML. The different surface morphologies [(2×2), missing-row reconstruction and (1×2) with 0.25 ML disordered copper vacancy] have comparable energetics and no energetically favorable site for oxygen embedment is predicted. To find the energetically favorable transition states on the missing-row reconstructed Cu(100) surface, we will investigate oxygen embedding paths with and without point defects on the top copper layer.

1Department of Energy Grant.

10:36AM A26.00010 Ab initio vibrational dynamics of Ag$_{27}$-Cu$_{17}$ nanoalloy. MARISOL ALCANTARA ORTIGOZA, University of Central Florida, ROLF HEID, KLAUS P. BOHNEN, Forschungszentrum Karlsruhe (IFP), TALAT S. RAHMAN, University of Central Florida — We have carried out calculations of the vibrational dynamics of the 34-atom nanoalloy, Ag$_{27}$-Cu$_{17}$, using density functional perturbation theory, which furnishes a powerful and reliable method to assess the linear response of the charge density to ionic perturbations. We find that the D$_{3h}$ core-shell structure of Ag$_{27}$-Cu$_{17}$ is dynamically stable, since all modes have non-zero frequencies affirming that the structure does not surrender itself to structural transitions as a result of the small perturbations in the charge density led by vibrations. The phonons of Ag$_{27}$-Cu$_{17}$ range from 2.6 to 28.5 meV and are relatively evenly distributed. There are, however, three ~3.0 meV gaps between 2.8-5.6, 15.0-18.7, and 23.6-26.8 meV. In modes whose frequency is below 7.0 meV, Ag atoms move the most while Cu atoms show a very small displacement. The opposite is true for four modes whose frequency is above 24 meV. We present the displacement patterns of the main modes and find the mode with highest energy to be a radial breathing mode of Cu atoms with respect to the center of the cluster. [1] G. Rossi et al., PRL, 93, 105503 (2004), [2] M. Alcántara Ortigoza and T. S. Rahman, PRB 77, 195404 (2008). Work supported in part by U.S. DOE under Grant DE-FG02-07ER46354.

10:48AM A26.00011 Clusters, Platelets, and Nanowires of Mo-S, and Their Assemblies. P. MURUGAN, Central Electrochemical Research Institute, Karakidu, T.N. India, VIJAY KUMAR, DR. Vijay Kumar Foundation, Gurgaon, India, Y. KAWAZOE, IMR, Tohoku Univ., Sendai, Japan, N. OTA, Hitachi Maxell Ltd., Tokyo, Japan — Nano-structures of Mo-S are useful for removal of S in petroleum industry, as solid state lubricants in space and tribo-lubricants for Pt-free fuel cell research. We study by first principles density functional calculations Mo-S nanoclusters, nanowires, their assemblies, and triangular nano-platelets all of which have been produced in laboratory. Mo-S clusters have Mo polyhedral structures and sulfur atoms cap this metal polyhedron. These structures have high stability due to strong Mo-Mo and Mo-S bonding. Some of the polyhedral clusters have non-zero magnetic moments due to the partially occupied 4d states in Mo atoms. Mo$_5$S$_8$ octahedral cluster has ultra-high stability and it could be condensed to form Mo-S nanowire or nanorod. However, for high $H_s$ contents, we show that triangular platelets become more stable. The Mo-S nanowires are good electronic conductors and are interesting for miniature devices. Assembly of nanowires stabilizes in a hexagonal structure with vdW interactions. The trigonal void between the nanowires can be occupied by Li atoms to develop materials for Li-ion battery applications. References: P. Murugan, V. Kumar, Y. Kawazoe, and N. Ota, Appl. Phys. Lett. (2008); Nano letters. (2007); J. Phys. Chem. A (2007).

Monday, March 16, 2009 8:00AM - 11:00AM — Session A27 GLMS: Focus Session: Advances in Scanned Probe Microscopy I: Low Temperatures 329

8:00AM A27.00001 Development of an Ultra Low Temperature Scanning Tunneling Microscope. YOUNG JAE SONG, ALEXANDER OTTE, NanoCenter, University of Maryland, College Park, MD/Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, Seoul, Korea, JOSEPH STROSCIO, Center for Nanoscale Science in Science and Technology, NIST, Gaithersburg, MD — In this talk we give an update on the next generation of ultra low temperature, high magnetic field (1ST) scanning tunneling microscope (STM). With this system, we plan to extend the capability of STM to include higher energy resolution (~1μeV) for scanning tunneling spectroscopy (STS) with operation at 20 mK. To realize this energy resolution in STS, we constructed an ultra high vacuum dilution refrigerator (DR) for STM applications. It operates with two independent modes of He3-He4 mixture gas condensation: a traditional 1K pot condenser, or a Joule-Thomson condenser for possible lower noise operation. This eliminates potential vibration problems during operation of the DR. To match the very low limit of thermal noise in this system, our new system includes extensive vibration isolation and RF shielding. Our STM sample holder has five isolated electrical contacts. This allows four-probe macroscopic electrical measurements to be performed simultaneously with microscopic STM measurements. The current progress and performance of this new system will be discussed.

8:12AM A27.00002 Design and construction of a millikelvin scanning tunneling microscopy system. MARK GUBRUD, Physics Dept., University of Maryland, College Park, BARRY BARKER, Laboratory for Physical Sciences, MICHAEL DREYER, DAN SULLIVAN, University of Maryland, College Park — We are developing a scanning tunneling microscopy and spectroscopy system for work at millikelvin temperatures, intended for studies of superconductor, semiconductor, and other materials and systems of interest to quantum computing research. Our approach incorporates recent advances in this field as well as original insights and innovations to help achieve low noise and low effective operating temperatures.

8:24AM A27.00003 Direct evidence of the surface state contribution to the Kondo resonance. QING LI, ISSP, Univ. Tokyo and Inst. Phys., CAS, SHIRO YAMAZAKI, TOYOAKI EGUCHI, ISSP, Univ. Tokyo, HOWON KIM, SE-JONG KAHNG, Dept. Phys., Korea Univ., JINFENG JIA, QIKUN XUE, Inst. Phys., CAS and Tsinghua Univ., YUKIO HASEGAWA, ISSP, Univ. Tokyo — We performed low temperature scanning tunneling microscopy/spectroscopy on the isolated single 5, 10, 15, 20-tetrakis-(4-bromophenyl)-porphyrin-Co (TBrPP-Co) molecules adsorbed on the Si(111): √3 x √3 Ag substrate. On this substrate, all the TBrPP-Co molecules show a square shape, indicating a planar conformation with a spin-active Co atom caged at its center. As the substrate supports a two-dimensional surface state and does not have bulk state near the Fermi level, the observed Fano-shaped peak near to the Fermi level is a direct evidence of the contribution of the surface state electrons to the Kondo resonance. The long decay length (∼ 1.4 nm) of the resonance also support for the surface state contribution. [1] Q. Li, S. Yamazaki, T. Eguchi, Y. Hasegawa, H. Kim, S.-J. Kahng, J. F. Jia, and Q. K. Xue, Nanotechnology 19, 465707 (2008).
8:36AM A27.00004 Kondo Effect in a Co-Porphyrin on Au(111) probed by Scanning Tunneling Spectroscopy. SE-JONG KAHNG, HOWN KIM, WON JUN JANG, JUNG HEUM JEON, Korea University, WON-JOON SON, SEUNGWU HAN, Ewha Womans University — Kondo effect is a core topic in condensed matter physics, exhibiting a localized state raised by the interaction between a single magnetic impurity and Fermi electrons in metals. We have studied Kondo effect in a Co-porphyrin on Au(111) using low-temperature scanning tunneling spectroscopy. A localized state is observed at Fermi level from the spectra measured above the Co atom. The spectra were fitted by Fano line shape, revealing the Kondo temperature of the system ~ 400K. By taking spectra at points along some symmetry directions, decaying behavior of the Kondo effect could be analyzed. With the help of simulated d-electron orbital, the observed decaying behavior is accounted for. Our study implies that lattice reconstruction in a system can induce d-electron orbital distortion, resulting in magnetic asymmetries.

8:48AM A27.00005 Imaging the Quantum Berry Phase. C.R. MOON, L.S. MATTOS, B.K. FOSTER, H.C. MANOHARAN, Department of Physics, Stanford University — Geometric phase operations are attractive to quantum information technology because they are time-independent and relatively insensitive to topological perturbations. However, in most coherent devices where these operations could be performed, electron wave functions are inaccessible to local probes. Here, we demonstrate Berry phase rotations on two-dimensional electron wave functions by using atomic manipulation to adiabatically alter their confinement potential. By consecutively changing the boundary of a quantum corral, we traverse a closed circuit in deformation space that engenders a net phase shift in two electron eigenstates. With scanning tunneling microscopy, we trace both the energetic and spatial evolution of these states and directly track their accrual of geometric phase, revealing information that would be obscured in other two-dimensional electron devices. This enables the determination of the two-point transconductance through the device, thus making contact to other nanostructures such as semiconductor quantum dots, where this promising technique for phase control can be implemented using only voltages controlling appropriately patterned gates.

9:00AM A27.00006 Evolution of Single-Molecule Vibrational Modes from Tunneling to Quantum Point Contact. W. MAR, W. KO, C. R. MOON, B. K. FOSTER, L. S. MATTOS, H. C. MANOHARAN, Stanford University — A detailed understanding of how molecular junctions form and evolve is vital for emerging fields such as molecular electronics. We present high-precision scanning tunneling microscopy studies tracing the evolution of molecular junctions from the tunneling regime to quantum point contact. We employ a model system of CO molecules on Cu(111) and are able to extend inelastic spectroscopy into the point contact regime, thus following the energy shifts of specific vibrational modes as the molecular contact is formed. We observe surprising non-monotonic shifts, confirmed by simultaneous noise measurements traceable to molecular motion. In point contact, we also observe a novel “nucleonic gating” effect in which the carbon nucleus controls a measurable dc molecular conductance shift. This shows that the electrical properties of molecular wires can be profoundly altered by their isotopic makeup. We extend these measurements to geometries where the three-dimensional approach vector of the tip relative to the target molecule is finely controlled, a technique not possible in break junction measurements.

9:12AM A27.00007 Low Temperature Scanning Tunneling Microscopy of High Temperature Superconductors: What We Gain By Taking a Closer Look. ERIC HUDSON, MIT — Scanning tunneling microscopy (STM) and spectroscopy have been applied to a wide variety of experimental systems. In this talk I will focus on one which was discovered at nearly the same time as STM — high temperature superconductors. After two decades of intense research these materials still hold many mysteries, mainly due to the rich variety of states of matter that may coexist, cooperate, or compete with superconductivity. I will present the unique perspective that STM is capable of bringing to our study of these materials through atomic-scale temperature dependent mapping of the density of states. After describing widely observed spatial “checkerboard” patterns which we have found to have a distinct doping dependence suggestive of charge density wave order, I will demonstrate how local variations of this order can help us understand nanoscale inhomogeneity in these materials. Taken together, these results not only show the power of STM to untangle complex nanoscale phenomena but also suggest a new path towards understanding high temperature superconductivity.

9:48AM A27.00008 Vortex excitation in nano-sized Pb island structures using low temperature scanning tunneling microscopy. TAKAHIRO NISHIO, ISSP, Univ. Tokyo, SHIZENG LIN, WPI-MANA, NIMS, KOUSUKE MIYACHI, TOSHI AN, TOYOAKI EGUCHI, YUKI HIHARCANA, ISSP, Univ. Tokyo — Vortex behaviors in nano-size superconductors have attracted a lot of attention since there are various novel phenomena due to the size and shape effects. Using scanning tunneling microscopy/spectroscopy (STM/S) at low temperature (<2 K) we have visualized vortex phases on atomically-flat nano-sized Pb islands formed on the Si(111)-(7×7) substrate and measured the critical magnetic fields for vortex penetration and expulsion [1]. In this study we demonstrate the excitation of a vortex with additional pulsed tunneling current from an STM probe tip. We found that probability of the excitation depends on the amount of the tunneling current, the pulse duration and a tip position in the island. These dependences suggest that the formation of normal state region below the tip due to the excess tunneling current induces the vortex penetration. Experimental details and theoretical results will be explained in the presentation. [1] T. Nishio et al., PRL 101, 167001(2008).

10:00AM A27.00009 Spatial and temperature-evolved tunneling spectroscopic studies of La0.5Ca0.5MnO3( LCNO) films and LCNO/organic-semiconductor heterostructures with spin-polarized scanning tunneling microscopy (SP-STM). C.R. HUGHES, A.D. BEYER, N.-C. YEH, Phys. Dept., Caltech, Pasadena CA — We report studies of spatially resolved tunneling spectra (TS) of La0.7Ca0.3MnO3 (LCMO) (Tc = 260K) epitaxial films and related heterostructures of tris(8-hydroxyquinoline) aluminum (Alq3)/(LCMO) using a UHV, variable temperature STM. At 77K with a Pt/Ir tip we observe sharp transitions between two cluster types with disparate normalized conductance. The majority type region exhibits high conductance peaks at high bias (+/- 2V) and a low energy gap, consistent with band structure calculations. The minority type region reveals moderate conductance over the entire bias range, from -3V to +3V. In contrast, spin-polarized tunneling spectra taken with Cr-coated STM tips show a spatially varying low bias gap in all regions. Further experiments using SP-STM on LCNO under varying temperatures and applied magnetic fields and on Alq3/LCNO structures to study the spin transport length in Alq3 will be reported.

1Supported by NSF and the Research Corporation.

This work was supported by NSF under Caltech/CSEM.
10:12AM A27.00010 Degeneracy lifting of zero energy (Majorana) modes in a chiral p-wave superconductor due to the tunneling between vortices.¹, MENG CHENG, ROMAN LUTCHYN, VICTOR GALITSKI, SANKAR DAS SARMA, University of Maryland — We study lifting of the degeneracy of the zero energy (Majorana) modes in a chiral $p_x + ip_y$ superconductor caused by tunneling between states localized in two different vortex cores. Using Bogoliubov-de Gennes equations, we analytically calculate the energy splitting of the Majorana modes as a function of the distance between two vortices. Our result may have applications in testing Majorana state by tunneling spectroscopy and the realization of topological quantum computation in chiral p-wave superconductors.

¹This work was supported by JQI and ARO-DARPA

10:24AM A27.00011 The role of magnetic anisotropy in the Kondo effect. ALEXANDER OTTE, NIST, MARKUS TERNES, IBM Research, KIRSTEN VON BERGMANN, Universitaet Hamburg, SEBASTIAN LOTH, IBM Research, HARALD BRUNE, EPFL, CHRISTOPHER LUTZ, IBM Research, CYRUS HIRJIBEHedin, University College London, ANDREAS HEINRICH, IBM Research — The Kondo effect is a fascinating many-body phenomenon, the origin of which is often unclear. Using a Scanning Tunneling Microscope operating at 0.5 K, we study inelastic spin excitations on individual atoms bound atop a thin insulating Cu$_2$N layer. We find that, unlike previously studied Fe and Mn atoms, the spins of Co and Ti atoms are Kondo screened in this environment. By applying strong magnetic fields in various directions we are able to precisely analyze the magneto-crystalline anisotropy experienced by the spins, and consequently their orientations relative to the surface. We show that the anisotropy plays a major role in determining whether or not a spin becomes Kondo screened, and how the Kondo effect is influenced by a magnetic field.

10:36AM A27.00012 Tunneling through a single magnetic atom: spin-dependent elastic and inelastic processes. C.F. HIRJIBEHEDIN, A. MODY, X. SHI, A. FISHER, London Centre for Nanotechnology, Dept. of Physics & Astronomy, Dept. of Chemistry, UCL, A.F. OTTE, NIST, M. TERNES, S. LOTH, C.P. LUTZ, A.J. HEINRICH, IBM Research Division, Almaden Research Center — Recent low-temperature scanning tunneling microscopy and spectroscopy studies have used inelastic electron tunneling to probe the spin excitations of magnetic atoms, molecules, and bulk surfaces. Here we describe the mechanisms that drive these spin excitations using a combination of resonant two-step and three-step virtual processes, with the latter including a simple exchange coupling between the tunneling electron and the electrons that comprise the atomic spin. Our description predicts the existence of a sum rule that includes a previously unnoticed type of spin-dependent elastic scattering, and evidence of both are seen in the observed spectra. We discuss the key factors that determine the relative strength of the inelastic tunneling, providing insight on when such processes can be observed and potentially how they might be enhanced.

10:48AM A27.00013 Implementation of a cryogenic scanning microwave impedance microscope. KEJILAI, WORASOM KUNDHIKANJANU, MICHAEL KELLY, ZHI-XUN SHEN, Stanford University — We have implemented a near-field scanning microwave impedance microscope in a variable temperature (2-300K) cryostat equipped with 9T magnet. Reflected microwave signals at 1GHz from a shielded cantilever probe were detected using room-temperature electronics. During the tip-sample approach, a small oscillating voltage was applied to the z-piezo and the modulated microwave signals were monitored to locate the sample surface. The approaching curve toward bulk dielectric materials can be quantitatively simulated by finite-element analysis. We have obtained the first low-T and high-B microwave images on a patterned silicon wafer with ion-implanted stripes. The results show clear impedance contrast in both the capacitive and loss channels. In particular, high-B regions were seen between the heavily doped areas and the insulating substrate, allowing us to visualize the local conductivity variation. With this novel instrument, we expect to study electronic inhomogeneity in complex materials and explore local properties during phase transitions.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A28. FIAP: Bionanotechnology 330

8:00AM A28.00001 Mesoscopic light reflection spectroscopy of weakly disordered dielectric media: Nanoscopic to mesoscopic light transport properties of a single biological cell and ultra-early detection of cancer. PRABHAKAR PRADHAN, HARIHARAN SUBRAMANIAN, DHWANIL DAMANIA, HEMANT ROY, VADIM BACMAN, Northwestern University, Evanston, IL 60208 — We have developed a mesoscopic partial wave spectroscopy (PWS) method to measure the nanoscopic light transport properties of weakly disordered dielectric mesoscopic systems such as biological cells. Using mesoscopic theory, we have statistically quantified the light reflection coefficient and its correlation due to nanoscale refractive index fluctuations within a biological cell, and the results are consistent with the prediction of mesoscopic light transport theory. Finally, using these parameters, we have characterized the nanoscale optical disorder strength within the biological cell. Results of precancerous cell studies and cancer detection by the technique will be discussed.

8:12AM A28.00002 Stick-Slip Motion of DNA in a Solid Nanopore¹. BINQUAN LUAN, GLENN MARTYNA, IBM TJ Watson Research Center — Nanopore technology is a potential solution for the low-cost and high-throughput DNA sequencing. Till now, in a typical experiment DNA driven by an electric field translocates through a nanopore too fast to be detected at a single-base resolution. The recently proposed DNA transistor (Appl. Phys. Lett. 91, 153103 (2007)) holds the promise to trap DNA inside a nanopore and translocate single-stranded DNA (ssDNA) at a single-base resolution. Using extensive all-atom molecular dynamics simulations, we modeled the process of ssDNA’s translocation through the DNA transistor when ssDNA is pulled by an optical tweezer. We found a stick-slip type of motions of DNA when both the stiffness of an optical tweezer and the pulling velocity are below critical values. This irregular motion of DNA is quantitatively characterized using the Tomlinson model. In a typical slip event, ssDNA advances one nucleotide and relaxes, while in a stick state the base of DNA can be conveniently measured. The duration of a stick state depends on the stiffness of a trapping field in the DNA transistor, the stiffness of an optical tweezer and the pulling velocity. Therefore, the controlled stick-slip motion of DNA is ideal for DNA sequencing methods using a solid nanopore.

¹Authors acknowledge the usage of IBM Bluegene supercomputers.

8:24AM A28.00003 Ionic Dependence of the Conformation and Dynamics of DNA Confined in Slit-like Nanofluidic Channels. YONGQIANG REN, WALTER REISNER, DEREK STEIN, Brown University — Due to the growth in nanobiological technology for DNA manipulation and analysis there is growing interest in understanding the physics of DNA in nanoconfined environments. Using fluorescence video microscopy we study the ionic dependence of static and dynamic properties of DNA molecules confined in slit-like nanofluidic channels with varying channel height. We observe an abrupt transition from the de Gennes regime to the Odijk regime for different ion concentrations for both the radius of gyration and the relaxation time. The cross-over channel height between the regimes increases with decreasing ionic strength. By direct measurement of the distribution function for the radius of gyration we can clearly show that the DNA molecules perform 2-D self-avoiding random walks for both the de Gennes and Odijk regimes. We also investigate the possible effects of electrostatic DNA-channel wall interactions.
Development of a nanopore-based electrical device for controlling the translocation of DNA with single base resolution and mass-production methods for sub-5 nm nanopores. WALTER REISNER, Dept. of Physics, Brown University, NIELS LARSEN, ANDERS KRISTENSEN, DTU Nanotech - Dept. of Micro- and Nanotechnology, Technical University of Denmark, JONAS O. TEGENFELDT, Department of Physics, Division of Solid State Physics, Lund University, HENRIK FLYVBÆRJ, DTU Nanotech - Dept. of Micro- and Nanotechnology, Technical University of Denmark — We have developed a new DNA barcoding technique based on the partial denaturation of extended fluorescently labeled DNA molecules. We partially melt DNA extended in nanofluidic channels via a combination of local heating and added chemical denaturants. The melted molecules, imaged via a standard fluorescence videomicroscopy setup, exhibit a nonuniform fluorescence profile corresponding to a series of local dips and peaks in the intensity trace along the stretched molecule. We show that this barcode is consistent with the presence of locally melted regions and can be explained by calculations of sequence-dependent melting probability. We believe this melting mapping technology is the first optically based single molecule technique sensitive to genome wide sequence variation that does not require an additional enzymatic labeling or restriction scheme.

Translocation Studies of Single Strand-DNA Oligomer Complexes with ds-DNA Markers Using Solid-State Nanopores. VENKAT BALAGURUSAMY, PAUL WEINGER, SUNGCHEOL KIM, XINSHENG SEAN LING, Brown University — We have designed short oligomers of single strand DNA of about 130 bases long each with 12-bases long sticky ends that are complimentary to those on one end of other oligomers to form ds-DNA regions by Watson-Crick base-pairing in these regions. Such a design facilitates the formation of a chain of single strands of DNA with ds-DNA regions interspersed. In order to slow down the translocation speed of these complexes through solid-state nanopores that could enable one to identify the ds-DNA region markers in the blockage current signal during translocation, we have attached these ss-DNA complexes with a polystyrene bead on one end. We present the results of our preliminary studies that show that the signature of these ds-DNA region markers could be identified.

Magnetophoresis of Fe$_3$O$_4$ Nanorods. DAVID TAN, JITKANG LIM, CAITLIN LANNI, FREDERICK LANNI, ROBERT TILTON, SARA MAJETICH, Carnegie Mellon University — The magnetophoretic motion of a nanorod is quite different from that of a nanosphere. In large particles, motion is predicted from the balance of magnetic and viscous drag forces, but for nanoparticles random thermal forces lead to Brownian motion as well. Due to magnetic and diffusive anisotropy, a nanorod has advantages over a nanosphere for the single particle guidance and tracking, which would be important for studies within living cells. We have investigated the magnetophoretic behavior of nanorods and nanospheres both theoretically and experimentally. Peclet number analysis shows that 300 nm x 20 nm nanorods are more likely to be in the convective than diffusive regime than nanospheres of equal volume, for the same field and field gradient. Experimental studies of nanorod motion were made using Fe$_3$O$_4$ nanorods coated with poly(diallyldimethylammonium chloride) and fluorescein-S-i-sothiocyanate (FITC) tagged bovine serum albumin (BSA) and dispersed in saline solution. The motion of the nanorods was observed with and without magnetic field gradients using fluorescence microscopy. Fluorescence micrograph showed the nanorods undergo magnetophoretic motion toward the higher field gradient region with a velocity of about 28µm/sec. The controlled motion of magnetic nanorods within HeLa cancer cells has been demonstrated.

Chip-based Magnetic Resonance System for Medical Diagnosis. HAKHO LEE, TAE-JONG YOON, RALPH WEISSLEDER, Massachusetts General Hospital/ Harvard Medical School — We have developed a chip-based, diagnostic magnetic resonance (DMR) system that can perform rapid, quantitative and multi-channeled detection of biological targets. The measurement is based on the effect of molecularly targeted magnetic nanoparticles on NMR (nuclear magnetic resonance) signals. With magnetic nanoparticles bound to their intended detection targets, the overall spin-spin relaxation time of bulk samples will be significantly shortened, as the particles efficiently dephase spins of surrounding water protons. Because the signal detection relies on NMR, the interference from media becomes negligible, making it possible to perform measurements in native biological samples (e.g., blood, sputum and urine). As proof of concept, we have developed a first DMR prototype by integrating microcups, microfluidic channels and a permanent magnet. The microcups, used as an NMR probe, are arranged in an array format for multiplexed, parallel detection. The microfluidic channels provide on-chip mixing between magnetic nanoparticles and biological samples and confine the mixture to microcups for high filling factor. Here, we demonstrate clinical utility of the DMR system by measuring proteins at exquisite sensitivities (~1 pM), identifying the disease condition of human sera, and profiling cancer cells according to their cell-surface markers.

Hyperpolarized Long-T$_1$ Silicon Nanoparticles for Magnetic Resonance Imaging. MAJA CASSIDY, SEAS, Harvard University, MA, JACOB APTEKAR, ALEXANDER JOHNSON, ROBERT BARTON, MENYOUNG LEE, ALEXANDER OGIER, CHINH VO, Department of Physics, Harvard University, MA, CHANDRASEKHAR RAMANATHAN, DAVID CORY, Department of Nuclear Science and Engineering, MIT, MA, ALISON HILL, ROSS MAIR, MATTHEW ROSEN, RONALD WALSWORTH, Harvard-Smithsonian CfA, MA, CHARLES MARCUS, Department of Physics, Harvard University, MA — Nanoparticles are currently being widely investigated as targetable contrast agents for magnetic resonance imaging (MRI). Silicon is a promising material system for use as a magnetic resonance imaging agent due to its long bulk (T$_1$) times and receptivity to hyperpolarization. We present studies of the nuclear relaxation (T$_1$) times of silicon nanoparticles as a function of particle size, dopant concentration and fabrication method. The T$_1$ times of these particles are found to be remarkably long (depending on size and dopant concentration), allowing for them to be transported and administered on practical timescale. In addition, we discuss the particles' receptivity to hyperpolarization, via low temperature microwave induced dynamic nuclear polarization.

This work is supported by grants from NIH and NSF.

This work is supported by the NIH under grant no. 1 R21 EB007486-01A1 and the Harvard NSEC.
9:48AM A28.00010 Magnetic detection of biotin-streptavidin binding using InAs quantum well \( \mu \)-Hall sensor, KALED ALEDEALAT, K. CHEN, Department of Physics and MARTECH, Florida State University; G. MIHAJLOVIC, Materials Science Division, Argonne National Laboratory, P. XIONG, Department of Physics, MARTECH and INSI, Florida State University, S. VON MOLNÁR, Department of Physics, MARTECH and INSI, Florida State University, M. FIELD, G.J. SULLIVAN, Teledyne Scientific Company LLC — Magnetic sensors are a key component in any high-sensitivity, rapid-response, and portable platform for magnetic biosensing. InAs quantum well micro-Hall sensors have shown high potential for such a role due to their low noise level and capability to detect single micron-sized or smaller superparamagnetic beads suitable for biosensing. Here we present successful selective biotinylation of InAs micro-Hall sensors and directed self-assembly of 350 nm streptavidin-coated superparamagnetic beads via the biotin-streptavidin interaction. Two Hall crosses with three and two beads produced detection signals with S/N ratio of 21.3 dB and 18.4 dB respectively. In addition, our progress for \( \textit{in situ} \) detection of micron-sized magnetic beads using microfluidic channel will be presented. 1 G. Mihajlovic et al., APL 87, 112502 (2005) This work was supported by NIH NIGMS GM079592.

10:00AM A28.00011 Single Nanometric Memory Unit Based On a Protein-Nanoparticle Hybrid, IZHAR MEDALYS, Physical Chemistry department, The Hebrew University, Jerusalem, 91904, Israel, ARNON HEYMAN, ODED SHOSEYOV, The Faculty of Agriculture, The Hebrew University, Rehovot 76100, Israel, DANNY PORATH, Physical Chemistry department, The Hebrew University, Jerusalem, 91904, Israel — Proteins as an isolating template and nanoparticle (NP) as an electric storage component can form a single addressable unit cell isolated from the conductive surface and adjacent NPs. This setup gives rise to a wide range of nanoelectronic applications. Here we demonstrate, by Conductive AFM, a single nanometric memory unit using individual protein-NP hybrids. SP1 is a boiling-stable ring-shaped protein, 11 nm in diameter. Mutants of SP1 were synthesized allowing its selective attachment to gold surface and the formation of 2D arrays using methods such as phospholipids trough and Langmuir Blodgett. The SP1 inner pore was connected to Si NP forming a chargeable entity embedded in an isolating unit over a conductive surface. Each NP holds three charging states: natural, positive and negative. The charging life times are 10 min in ambient and days in vacuum. Using this setup, and the relative long charging time, we were able to apply a read and write operations on individual 5nm Si NP embedded in a stable protein.

10:12AM A28.00012 Characterization of the Uptake of Quantum Dots by Algae, PRIYANKA BHATTACHARYA, SIJIE LIN, Department of Physics and Astronomy, Clemson University, XIAOQIAN SUN, Department of Mathematical Sciences, Clemson University, DAVID BRUNE, Department of Agricultural and Biological Engineering, Clemson University, PU-CHUN KE, Department of Physics and Astronomy, Clemson University — The exposure of living systems to nanoparticles is inevitable due to a dramatic increase in their release into the environment, the most likely pathways being through inhalation, ingestion and skin uptake. The extremely small size of the nanoparticles may facilitate their tissue and cellular uptake by plants and animals, resulting in either positive (drug delivery, antioxidation) or negative (toxicity, cellular dysfunction) effects. Here we report the effects of quantum dots uptake by algae, the single-celled plant species and major food sources for aquatic organisms. In our studies, the presence of quantum dots in algal cells was detected using fluorescence microscopy and electron microscopy. Using spectrophotometry we found a supralinear increase of the uptake with the concentration of quantum dots, with a saturation of the uptake occurring beyond a concentration of 15 mg/mL. Using a bicarbonate indicator we further evaluated the effects of quantum dots uptake on algal photosynthesis and respiration. Such study facilitates our understanding of the environmental impact of nanomaterials.

1 PCK acknowledges NSF grant CBET-0736037 and NSF Career award CBET-0744040.

10:24AM A28.00013 Thermochemical nanolithography of multi-functional templates for selective assembly of bioactive proteins, DEBIN WANG, VAMSI KODALI, WILLIAM UNDERWOOD, JONAS JARVHOLM, TAKASHI OKADA, SIMON JONES, MARIACRISTINA RUMI, ZHENTING DAI, WILLIAM KING, SETH MARDER, JENNIFER CURTIS, ELISA RIEGO — Atomic force microscopy based techniques have been successful in generating protein nano-arrays on various substrates. However, several challenges still exist in terms of resolution, writing speed, cost, substrate choice, protein bioactivity, multi-component patterning, and surface passivation. Recently, we have developed the use of thermochemical nanolithography combined with post covalent functionalization and molecular recognition on a polymer surface of a single chip to produce multiplexed nanopatterns at speeds of mm/s. These patterns can then be functionalized under native conditions to create tailored nano-assemblies of two different species of proteins coexisting on the same surface. The proteins attach selectively and strongly to the nanopatterns via covalent and/or specific interactions, while retaining their ability to interact specifically with other proteins in buffered solution. At present, this method has produced nanopatterns of bio-active proteins with features as small as 40 nm on polymer films. This technique opens up new possibilities in nanoscale manipulation of biological macromolecules as well as many molecular biophysics studies such as inter-protein interactions.

10:36AM A28.00014 Directional Growth of Polymeric Nanowires, PREM THAPA, BRETT FLANDERS — This work establishes an innovative electrochemical approach to the template free growth of conducting polypyrrole and polystyrene wires. These polymeric wires exhibit a knobby structure, but persistent growth in a given direction up to 30 \( \mu \)m in length. A long-range component of the applied voltage signal defines the growth-path. Moreover, the presence of this component enables the growth of amorphous nanowires with wire-like geometries. Such wires are employed in a non-invasive methodology for attaining strong mechanical attachments to live cells. This capability is of potential use in the electro-mechanical probing of cell physiological processes.

10:48AM A28.00015 A novel nanoarchitecture with optical, solar, medical and biochemical utility, M.I. NAUGHTON, K. KEMP, Z.F. REN, Boston College and Solasta Inc. — We discuss a nanoscale platform offering widespread utility in nanophotonics, photovoltaics, visual prosthetics, and biological and chemical sensing. As a subwavelength wave-guide architecture, these nanostructures can be used in array form for high efficiency solar cells, as well as in a wide range of nanoscale manipulations of light without deleterious plasmonic effects. They are also being developed as a high-electrode-density (10^9/cm^2) retinal implant. Finally, a modification of the basic structure enables the fabrication of a highly sensitive “nanocavity” biochemical sensor. We will report on aspects of each application. We also thank the following collaborators: N. Argenti, D. Cai, T.C. Chiles, P. Dhakal, Y. Gao, T. Kirkpatrick, Y.C. Lan, G. McMahon, J.J. Oh, B. Rizal, J. Rybczynski.

1 Portions of this work are supported by NSF, DOE and Solasta Inc.

Monday, March 16, 2009 8:00AM - 11:00AM —
Session A29 GMAG: Spin Glasses and Disordered Magnetic Materials 333
8:00AM A29.00001 Probing the relation between structural glasses and 3-spin glass phases using one-dimensional models . DEREK LARSON, Physics Dept., University of California Santa Cruz, Santa Cruz CA 95064; HELMUT G. KATZGRABER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland; Department of Physics, Texas A&M University, College Station, TX 77843-4242; A.P. YOUNG, Physics Dept., University of California Santa Cruz, Santa Cruz CA 95064 — Motivated by a proposed connection between 3-spin glass phases and structural glasses, we have performed Monte Carlo simulations on a one-dimensional long-range Ising glass with power-law interactions involving 3-spins. Varying the exponent of the power-law interactions is analogous to changing the space dimension of a corresponding short-range 3-spin model. We present results of a finite-size scaling analysis of the two-point correlation length, and compare our results with the prediction of Moore and Yeo that the three-spin model is in the same universality class as an Ising spin glass in a magnetic field.

8:12AM A29.00002 Study of the de Almeida-Thouless line using power-law diluted one-dimensional Ising spin glasses . HELMUT G. KATZGRABER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland; Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA; DEREK A. LARSON, A.P. YOUNG, Department of Physics, University of California, Santa Cruz, CA 95064, USA — We test the existence of a spin-glass state in an externally-applied (random) magnetic field via Monte Carlo simulations of a power-law diluted one-dimensional Ising spin glass. The model has the advantage over conventional short-range models in that by tuning the exponent of the power-law interactions we are able to scan the full range of possible behaviors from the infinite-range to the non-mean-field regime. Furthermore, due to the average fixed connectivity very large linear system sizes can be studied. An analysis of the two-point correlation length shows that the system in the non-mean-field universality class does not order in a field. This suggests that there is no de Almeida-Thouless line for short-range Ising spin glasses below the upper critical dimension.

8:24AM A29.00003 Reentrant and Forward Phase Diagrams of the Anisotropic Three-Dimensional Ising Spin Glass . CAN GÜVEN, A. NIHAT BERKER, Koç University, Michael Hinczewski, Technical University of Munich, Hidetoshi Nishimori, Tokyo Institute of Technology — The spatially uniaxially anisotropic d=3 Ising spin glass is solved exactly on a hierarchical lattice.[1] Five different ordered phases, namely ferromagnetic, columnar, layered, antiferromagnetic, and spin-glass phases, are found in the global phase diagram. The spin-glass phase is more extensive when randomness is introduced within the planes than when it is introduced in lines along one direction. Phase diagram cross-sections, with no Nishimori symmetry, with Nishimori symmetry lines, or entirely imbedded into Nishimori symmetry, are studied. The boundary between the ferromagnetic and spin-glass phases can be either reentrant or forward, that is either receding from or penetrating into the spin-glass phase, as temperature is lowered. However, this boundary is always reentrant when the multicritical point terminating it is on the Nishimori symmetry line. [1] C. Güven, A.N. Berker, M. Hinczewski, and H. Nishimori, Phys. Rev. E 77, 061110 (2008).

8:36AM A29.00004 The Blume-Emery-Griffiths Spin Glass and Inverted Tricritical Points . V. ONGUÖZÇELIK, A. NIHAT BERKER, Koç University — The Blume-Emery-Griffiths spin glass is studied by renormalization-group theory in d=3.[1] The boundary between the ferromagnetic and paramagnetic phases has first-order and two types of second-order segments. This topology includes an inverted tricritical point, first-order transitions replacing second-order transitions as temperature is lowered. The phase diagrams show disconnected spin-glass regions, spin-glass and paramagnetic reentrances, and complete reentrance, where the spin-glass phase replaces the ferromagnet as temperature is lowered for all chemical potentials. [1] V.O. Özçelik and A.N. Berker, Phys. Rev. E 78, 031104 (2008).

8:48AM A29.00005 Quenched-Vacancy Induced Spin-Glass Order . GÜL GÜLPİNAR, Dokuz Eylül University, A. NIHAT BERKER, Koç University — The ferromagnetic phase of an Ising model in d=3, with any amount of quenched antiferromagnetic bond randomness, is shown to undergo a transition to a spin-glass phase under sufficient quenched bond dilution.[1] This general result, demonstrated here with the numerically exact renormalization-group solution of a d=3 hierarchical lattice, is expected to hold true generally, for the cubic lattice and for quenched site dilution. Conversely, in the ferromagnetic-spin-glass-antiferromagnetic phase diagram, the spin-glass phase expands under quenched dilution at the expense of the ferromagnetic and antiferromagnetic phases. In the ferro-spin-glass phase transition induced by quenched dilution reentrance is seen, as previously found for the ferro-spin-glass phase transition induced by increasing the antiferromagnetic bond concentration. [1] G. Gülpınar and A.N. Berker, arXiv:0811.0025v1 [cond-mat.dis-nn] (2008).

9:00AM A29.00006 Nonequilibrium spin glass dynamics with the Janus computer . DAVID VILLANES, Universidad Complutense de Madrid, F. BELLETTI, A. CRUZ, L.A. FERNANDEZ, A. GORDILLO-GUERRERO, M. GUIDETTI, A. MAIORANO, F. MANTOVANI, E. MARINARI, V. MARTIN-MAYOR, J. MONFORTE, A. MUÑOZ SUDUPE, D. NAVARRO, G. PARISI, S. PEREZ-GAVIRO, J.J. RUIZ-LORENZO, S.F. SCHIFANO, D. SCIRETTI, A. TARANCON, R. TRIPICCIONE, JANUS COLLABORATION — The out of equilibrium evolution of the Edwards-Anderson spin glass is followed for a tenth of a second, effectively halving the (logarithmic) temporal gap between previous simulations and experiments. In fact, we have been able to make safe predictions about the behavior at experimental times, using mild extrapolations. This work has been made possible by Janus, a special purpose computer designed by our collaboration. We have thoroughly studied the spin glass correlation functions and the growth of the coherence length for $L = \infty$ lattices in 3D, using $L = 24, 40$ lattices to check for finite size effects. We present clear evidence for a replica correlator. Our main conclusion is that these spin glasses follow non-coarsening dynamics, at least up to the experimentally relevant time scales.


9:12AM A29.00007 Chaotic Spin Correlations in Frustrated Ising Hierarchical Lattices . NESE ARAL, A. NIHAT BERKER, Koç University — Spin-correlations are calculated in frustrated hierarchical Ising models that exhibit chaotic renormalization-group behavior. [1] The spin-correlations, as a function of distance, behave chaotically. The far correlations, but not the near correlations, are sensitive to small changes in temperature or frustration, with temperature changes having a larger effect. On the other hand, the calculated free energy, internal energy, and entropy are smooth functions of temperature. The recursion-matrix calculation of thermodynamic densities in a chaotic band is demonstrated. The spectrum of Lyapunov exponents is calculated as a function of frustration. [1] N. Aral and A.N. Berker, arXiv:0810.4586v1 [cond-mat.dis-nn] (2008).

9:24AM A29.00008 Tunable domain pinning in a Random-Field Ising Ferromagnet . D. M. SILEVITCH, James Franck Institute/University of Chicago, G. AEPPLI, London Centre for Nanotechnology and Department of Physics and Astronomy, UCL, London, T.F. ROSENBAUM, James Franck Institute/University of Chicago — The diluted magnetic salt LiHo$_2$F$_4$, was shown recently [Nature 448 567-570 (2007)] to be the first ferromagnetic realization of the random-field Ising model, where the strength of the random fields can be tuned by an external magnetic field. These random-field effects can be used to continually and reversely vary the pinning potential of the magnetic domains, allowing us to tune the hysteretic behavior. Magnetization measurements reveal enhanced pinning in the random-field regime as well as a temperature-dependent crossover into a regime dominated by quantum fluctuations.
9:36 AM A29.00009 A strongly disordered spin glass and minimum spanning trees

THOMAS JACKSON, NICHOLAS READ, Yale University — We investigate the ground state structure of a strongly disordered spin glass model proposed by Newman and Stein (NS). In the strong disorder limit, frustration is negligible and the problem of identifying ground states is equivalent to the minimum spanning tree (MST) problem in combinatorial optimization: given an edge-weighted graph, the MST is the subset of edges that connects all vertices, has no cycles, and minimizes the total edge weight. Here the weights are quenched random variables, and we use a relation between Kruskal's greedy algorithm for finding the MST and percolation. We solve this random MST on the Bethe lattice with appropriate boundary conditions, which defines a mean-field theory valid above \( d_c = 6 \) (NS proposed \( d_c = 5 \)). Above \( d_c \), NS showed that the spin glass model has infinitely many ground states, but only a single pair below \( d_c \). For \( d < d_c \), we develop a continuum field theory for the fractal dimension \( D_p \) of paths on the MST on critical percolation clusters; to first order in the epsilon expansion, we obtain \( D_p \approx 2 - (6 - d)/7 \) for \( d < 6 \) (\( D_p = 2 \) for \( d > 6 \)).

1Supported by NSF Grant No. DMR-0706195

9:48 AM A29.00010 ABSTRACT WITHDRAWN

10:00 AM A29.00011 Overlap as a Measure of Spin-Glass Memory and a Probe of Free Energy Landscape

WEN LUO1, University of Nebraska-Lincoln, MICHAEL MIHALCO, THOMAS E. STONE, SUSAN R. MCKAY, University of Maine — The degree of history dependence and the structure of the free energy landscape of the spin glass are both indicators of the complexity of this ordered phase. Using the Ising antiferromagnet on a triangular lattice, dilated with quenched random ferromagnetic bonds, we probe these indicators through repeated cycling between two temperatures. We consider cases in which both temperatures are within the spin-glass phase, and systematically vary the temperature difference between initial and final states. These results are compared with the same cycling pattern with one temperature inside and the other outside of the spin-glass phase. The overlap of the ground state for the former is non-zero even when the system remains within the spin-glass phase during cycling. A plot of the overlaps of the low temperature states and their differences in internal energy shows no simple relationship between overlap and internal energy. States with almost identical internal energies often have very little overlap.

1Supported by the University of Maine’s Research Experience for Undergraduates, funded by NSF/DoD Grant No. 0754951.

10:12 AM A29.00012 Quantum Effects for Interaction of Electron with coupled magnetic local spin chains

Fatih Dogan, University of Alberta, Edmonton, AB, Canada, Lucia Covacci, University of British Columbia, Wonkee Kim, University of Houston, Frank Marsiglio, University of Alberta — In this talk, we will look at time dependent interaction of an electron with ferromagnetic chain. We will show that ferromagnetic interactions between magnetic spins cause the electron interacting with them to change its energy and depending on the strength of interactions form a bound state. These effects are visible through the resulting state of the electron. Experimental suggestions will be given to observe this quantum behavior.

10:24 AM A29.00013 Avalanche Spatial Structure: Viewing Crackling Noise through Windows

Yan-Jun Chen, Stefanos Papanikolaou, James P. Sethna, LASSP, Cornell University, Gianfranco Durin, INRIM and ISI, Fondazione, Torino, Italy, Stefano Zapperi, INFN-CNR center, Modena, and ISI, Torino, Italy — In imaging experiments of Barkhausen noise in thin films, magnetic avalanches at the boundaries present challenges to analysis. Large avalanches are removed from the distribution, and the portion inside the viewing window may sometimes be treated as smaller avalanches. We analyze the scaling behavior of different categories of avalanches in artificially-windowed simulations of Barkhausen noise to examine the effect of window size on scaling relations. In passing, we discuss the average spatial shapes of avalanches, multivariable scaling functions, and the use of nonlinear-least-squares methods for exploring and reporting universal scaling functions.

10:36 AM A29.00014 Avalanche Average Shapes: Mean-field temporal average avalanche shape

Stefanos Papanikolaou, LASSP, Cornell Univ., Christopher R. Myers, Computational Biology Service Unit, Cornell Univ., Francesca Colaiori, CNR-INFN, Dipartimento di Fisica, Universita "La Sapienza", Roma, Karen E. Danielis, North Carolina State U., Gianfranco Durin, INRIM and ISI Foundation, Torino, Italy, Stefano Zapperi, INFN-CNR center, Modena and ISI in Torino, Italy, James P. Sethna, LASSP, Cornell Univ. — The average temporal shape of avalanches has been a fruitful application of universality and critical scaling, with experimental and theoretical investigations particularly in the field of magnetic Barkhausen noise. The mean-field shapes of these avalanches have been thought to come in two forms: inverted parabolas for the infinite-range model and one lobe of a sinusoid for the single-degree of freedom ABBM model. We show that the infinite-range model can be mapped onto the earlier ABBM model, and that the average shape for both mean field theories is an inverted parabola, seemingly resolving the ambiguity. However, we also propose a new mean-field model including the effects of local saddle-node bifurcations on the dynamics, and analyze both its predictions for dynamical exponents and temporal average shapes. We compare with experimental results on sheared granular materials.

10:48 AM A29.00015 Permutation Symmetric Critical Phases in Disordered Non-Abelian Anyonic Chains

Lukasz Fidkowski, Gil Refael, Hans-Hsuain Lin, Caltech, Paraj Titum, Indian Institute of Technology, Kanpur, India — Topological phases supporting non-abelian anyonic excitations have been proposed as candidates for topological quantum computation. We study disordered non-abelian anyonic chains below low-temperature quantum states provide a quantitative measure of the system’s memory, and is non-zero even when the system remains within the spin-glass phase during cycling. A plot of the overlaps of the low temperature states and their differences in internal energy shows no simple relationship between overlap and internal energy. States with almost identical internal energies often have very little overlap.

Monday, March 16, 2009 8:00 AM - 11:00 AM
Session A30 DMP GAM: Focus Session: Vanadates, Iridates and Other Oxides 334

8:00 AM A30.00001 Electronic band structure of metallic phase \( \text{V}_2\text{O}_3 \)

O. KRUPIN, J. DENLINGER, Lawrence Berkeley National Lab, B.J. KIM, RAVI S. SINGH, J.W. ALLEN, University of Michigan — \( \text{V}_2\text{O}_3 \) has an archetypal strongly correlated paramagnetic metallic (PM) phase which becomes insulating with alloying or decreasing temperature. Recent progress has been made experimentally to measure the true bulk V 3d density of states of PM phase \( \text{V}_2\text{O}_3 \) using high-energy angle-integrated photoemission, and theoretically to quantitatively describe the observed prominent quasiparticle peak near \( E_F \) using LDA+DMFT. Theoretical predictions of the \( k \)-resolved electronic band structure of \( \text{V}_2\text{O}_3 \) have been made, but experimental measurement has proven to be very challenging and elusive. We present intermediate-energy soft x-ray angle-resolved photoemission measurements of the PM-phase \( \text{V}_2\text{O}_3 \) (0001) cleaved surface that reveal for the first time distinct \( k \)-resolved band dispersions within the coherent quasiparticle peak and a corresponding three-fold symmetric Fermi surface topology. The agreement of these measurements to theoretical calculations will be discussed.

1Supported by the U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231) and at the University of Michigan (DE-FG02-07ER46379).
8:12AM A30.00002 Concurrent structural and magnetic phase transition in nanopowder V$_2$O$_3$. J. P. CARLO, Y. J. UEMURA, Department of Physics, Columbia University, New York, NY; V. BLAQOJEVIC, M. L. STEIGERWALD, L. E. BRUS, Department of Chemistry, Columbia University, New York, NY; S. L. BILLINGE, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY; W. ZHOU, Department of Physics, Michigan State University, Lansing, MI; G. M. LUKE, A. A. ACZEL, G. J. MACDOUGALL, Department of Physics and Astronomy, McMaster University, Hamilton, ON; P. W. STEPHENS, Department of Physics, SUNY at Stony Brook, Stony Brook, NY — V$_2$O$_3$, which has been the subject of investigations for well over 30 years, is a classic example of a Mott-Hubbard transition system. This first-order metal-insulator transition, near 160K, is accompanied by a rhombohedral-monoclinic structural as well as a paramagnetic-antiferromagnetic magnetic transition. We report on structural synchrotron x-ray characterization of V$_2$O$_3$ nanopowder (dia $\approx$ 10-50 nm) at NSLS, and magnetic characterization via muon spin relaxation at TRIUMF. We find that, just as in bulk V$_2$O$_3$, the structural and magnetic transitions are concurrent, and that in contrast to the abrupt and hysteretic transition witnessed in the bulk, in the nanopowder sample the transition occurs with phase separation over a broad temperature range.

8:24AM A30.00003 Metal-insulator transition in AV$_{10}$O$_{15}$ (A=Ba, Sr). T. KATSUFAJI, T. SUZUKI, T. KAJITA, Dept. Phys., Waseda Univ. — In AV$_{10}$O$_{15}$ (A=Ba, Sr), the V ions take a mixed-valence state, V$^{2.8+}$ (3d$^{2.2}$), and form a modified triangular lattice, in which V triangles are periodically missing from a normal triangular lattice. It is known that BaV$_{10}$O$_{15}$ undergoes a structural phase transition at around 120 K. We have succeeded in growing large single crystals of AV$_{10}$O$_{15}$ (A=Ba, Sr) by a floating-zone method. We found a large jump of electrical resistivity by $\approx 10^2$ times at the structural transition temperature (123 K) of BaV$_{10}$O$_{15}$, which can be regarded as a metal-insulator transition presumably dominated by a charge/orbital ordering of V. We also found an antiferromagnetic ordering at 43 K in the same compound. On the other hand, SrV$_{10}$O$_{15}$ did not show any structural anomaly down to the lowest temperature, and a spin-glass behavior was observed. These results indicate a strong correlation between the structural anomaly (charge/orbital ordering) and the magnetism in this series of compounds. We also measured the optical reflectivity of BaV$_{10}$O$_{15}$ and found the opening of a charge gap in the optical conductivity spectrum at low temperatures.

8:36AM A30.00004 Charge dynamics in thermally and doping induced insulator-metal transitions of (Ti$_{1-x}$V$_x$)$_2$O$_3$. MASAKI UCHIDA, JUN FUJIJKA, YOSHINORI ONOSE$^1$, YOSHINORI TOKURA$^2$, Department of Applied Physics, University of Tokyo — Charge dynamics of (Ti$_{1-x}$V$_x$)$_2$O$_3$ with $x = 0$–0.06 has been investigated by measurements of charge transport and optical conductivity spectra in a wide temperature range of 2–600 K with the focus on the thermally and doping induced insulator-metal transitions (IMTs). The optical conductivity peaks for the interband transitions in the 3d$^2$ manifold are observed in the both insulating and metallic states, while their large variation (by $\approx 0.4$ eV) with change of temperature and doping level scales with that of the Ti-Ti dimer bond length, indicating the weakened singlet bond in the course of IMTs. The thermally and V-doping induced IMTs are driven with the increase in carrier density by band-crossing and hole-doping, respectively, in contrast to the canonical IMT of correlated oxides accompanied by the whole collapse of the Mott gap.

$^1$also at Multiferroics Project, ERATO, Japan Science and Technology Agency (JST)
$^2$also at Multiferroics Project, ERATO, Japan Science and Technology Agency (JST) and Cross Correlated Materials Research Group (CMRG), ASI, RIKEN

8:48AM A30.00005 Intersite correlations and the metal insulator in cluster dynamical mean field theory: cluster size, interaction strength, and the location of the transition line$^1$, C. LIN, A. MILLIS, Columbia University — To gain insight into the physics of the metal insulator transition and the effectiveness of cluster dynamical mean field theory we have used one, two and four site dynamical mean field theory (both CDMFT and DCA) to solve a model of electrons coupled to a classical phonon field. A partial density of states is defined encoding a generalized nesting property of the band structure; variations in this density of states account for differences between dynamical cluster approximation and cellular-DMFT implementation of cluster DMFT, and for differences in behavior between single band (cuprate-like) and multiband (manganite-like) models. The cluster size dependence of the metal to polaronic insulator phase boundary is determined along with electron spectral functions and cluster correlation functions. Over most of the interaction strength regime the single-site and multi-site approximations are found to yield similar results. Important cluster size effects occur only in the metal insulator transition region, where short-ranged correlations are found to significantly reduce the critical interaction strength required to drive a metal polaron insulator transition. In the cluster approximations the physics of the metal-insulator transition is shown to be Slater-like (driven by band filling). The minimal cluster size required to capture the metal-polaron insulator transition is shown to depend sensitively on the carrier concentration. Implications for the theoretical treatment of doped manganites are discussed.

$^1$DOE-ER 46169 and Columbia MRSEC.

9:00AM A30.00006 Study of phase separated manganites by DC transport and infrared spectroscopy. A. ZIMMERS, T. WOLF, J. LESUEUR, R.P.S.M. LOBO, Laboratoire Photons Et Matiere, ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France; A. KUSHWAHA, R.C. BUDHANI, Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India — We present confined geometry measurements of manganites La$_{0.325}$Pr$_{0.1}$Ca$_{0.375}$MnO$_3$ (LPCMO) and La$_{2/3}$Sr$_{1/3}$MnO$_3$ (LSMO). As reported previously, due to electronic phase separation, LPCMO microwires show a step-like metal-insulator transition as temperature is lowered and as magnetic field is swept. We will show how this feature evolves as a function of the width and shape of the microwires. On the contrary, LSMO microwires are found to have a smooth transition in all wire sizes under a structural transition temperature (123 K) of LSMO, which has been investigated by measurements of charge transport and optical conductivity of the insulating and metallic states, while their large variation (by $\approx 0.4$ eV) with change of temperature and doping level scales with that of the Ti-Ti dimer bond length, indicating the weakened singlet bond in the course of IMTs. The thermally and V-doping induced IMTs are driven with the increase in carrier density by band-crossing and hole-doping, respectively, in contrast to the canonical IMT of correlated oxides accompanied by the whole collapse of the Mott gap.

9:12AM A30.00007 Spectral Function of Manganese Systems. JUAN SALAFRANCA, ELBIO DAGOTTO, Dept. of Physics and Astronomy, University of Tennessee and Materials Science and Technology Division, Oak Ridge National Laboratory — Using a double exchange model with Jahn Teller distortions, we calculate the one particle spectral function of manganese systems. The relative contribution of the different interactions is established by means of Monte Carlo and self consistent mean field calculations. In particular, we examine the effects of electron-electron and electron-phonon couplings. We discuss the relevance of our results in relation to recent Photoemission experiments on layered manganites [1], where similarities of manganites spectra with that of cuprates was observed.

9:24AM A30.00008 Anomalous nuclear relaxation in the ferromagnetic phase of the bilayered manganese La$_2$Sr$_6$Mn$_2$O$_9$... MICHAEL HOCH, PHILIP KUHNS, WILLIAM MOULTON, ARNEIL REYES, JUN LU, National High Magnetic Field Laboratory, 1800 E. Paul Dirac Dr., Tallahassee, FL 32310, JOHN MITCHELL, Argonne National Laboratory, Argonne, IL 60439 — In contrast to ferromagnetic (FM) 3D manganites, Mn NMR spectra obtained for the FM phase of the colossal magnetoresistance bilayer manganese La$_2$Sr$_6$Mn$_2$O$_9$ show a broad distribution of hyperfine fields implying a large distribution of local environments at Mn sites. The hyperfine distribution may be linked to orbital ordering effects. Mn spin – lattice relaxation rates have a surprisingly weak dependence both on temperature and applied magnetic field. Significant departures of the relaxation rate from Korringa temperature dependence below 20 K provide evidence for non-Fermi liquid behavior in this quasi-2D metal. At temperatures approaching $T_c$ from below, further anomalous behavior is found consistent with spin polaron formation in the range where colossal magnetoresistance starts to appear.

9:36AM A30.00009 Anomalous metallic state: Decisive effect of dilute impurity doping on ferromagnetic BaIrO$_3$ single crystals1, O.B. KORNETA, S. CHIKARA, T.F. QI, S. PARKIN, G. CAO, University of Kentucky, W.H. SONG, Institute of Solid State Physics, Hefei 230031, P.R. China — BaIrO$_3$ is a quasi one-dimensional system, where a CDW and a ferromagnetic state with $T_c$=183K coexist. The ground state of the system is critically linked to the lattice and orbital degrees of freedom due to extended 5d-orbitals. The central findings of this study are: (1) An occurrence of a 2D-metallic state with a linear temperature dependence of resistivity at low temperatures in slightly oxygen-deficient samples; (2) Unusual temperature dependence of resistivity above the Curie temperature in the rare-earth doped BaIrO$_3$; (3) High sensitivity of the resistivity to applied pressure (< 12 Kbar), which results in changes in resistivity by a few orders of magnitude in these doped samples. The results of the resistivity, heat capacity, magnetization, thermoelectric power and structural measurements as a function of temperature, magnetic field, and pressure will be presented and discussed. 

1 This work was supported by NSF grant DMR-0552267.

9:48AM A30.00010 Non-Fermi-liquid behavior in nearly ferromagnetic SrIrO$_3$ single crystals1, T.F. QI, S. CHIKARA, O.B. KORNETA, S. PARKIN, L.E. DE LONG, G. CAO, University of Kentucky, P. SCHLOTTMANN, Florida State University — We report magnetic, electric, transport, and calorimetric properties of single-crystal SrIrO$_3$ as a function of temperature $T$ and applied magnetic field $H$. We find that SrIrO$_3$ is a non-Fermi-liquid near a ferromagnetic instability, as characterized by the following properties: (1) small saturation moment and no evidence for long-range order down to 1.7 K, (2) strongly enhanced magnetic susceptibility that diverges as $T^3$ at low temperatures with $1/2 < \gamma < 1$, depending on the applied field, (3) heat capacity $C(T,H) \sim T^3/\ln T$ that is readily enhanced in low applied fields, and (4) $T^{1/2}$ dependence of electrical resistivity over the range 1.7 K $< T < 120$ K. The data imply SrIrO$_3$ is a rare example of a stoichiometric oxide compound that exhibits non-Fermi-liquid behavior near a quantum critical point ($T=0$ and $\mu_0H=0.23$ T). The results will be presented and discussed along with those of a similar system CaRuO$_3$.

1 This work was supported by NSF through grant DMR-0552267.

10:00AM A30.00011 Magnetic Soft Mode Behavior of the Field-Dependent Specific Heat of SrIrO$_3$. LANCE DE LONG, DAHENG HE, VINAYAK BHAT, GANG CAO, University of Kentucky — Previous work indicates SrIrO$_3$ is a strongly exchange-enhanced paramagnet (Wilson ratio = 75) exhibiting non-Fermi liquid (NFL) behavior at low magnetic fields, and a cross-over to weak ferromagnetism ($0.025 \mu_0$T/ir at $\mu_0H = 7.0$ T and $T = 1.7$ K) at applied fields $\mu_0H$ $\geq$ 3 T and temperatures $T$ $<$ 4 K. Measurements of the specific heat performed in constant field for 1.8 $<$ $T$ $<$ 4K have been used to extract the field dependence $C_p/(H,T)$ (constant $T_o$), which exhibits an Schottky-like peak as a function field in the range 1.0 $<$ $\mu_0H < 1.5$ T at increasing temperatures 1.8 $<$ $T_o$ $<$ 3.9 K, respectively. Fits of $C_p/(H,T_o)$ imply a nonmagnetic ground state is separated from magnetic excited states by an energy splitting $\Delta (H,T)/K_B$ $=$ $T^*$ that decreases from 7.5 to 2 K as $\mu_0H$ increases from 0 to 8 T. The Schotky peak field increases as $\mu_0H^2$ = 0.94 T + (0.03 T/K) $T^2$. We discuss how a semi-classical two-level model reproduces the NFL-weak ferromagnet cross-over with applied field.

2 Research supported by U.S. DoE Grant DE-FG02-97ER45653 and U.S. NSF Grant DMR-0552267.


10:12AM A30.00012 Temperature-dependent electronic structure evolution of spin-orbit coupling induced Mott insulator Sr$_2$IrO$_4$. S. J. MOON, W. S. CHOI, T. W. NOH, ReCOE and FPDR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, H. JIN, CSMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, Y. S. LEE, Department of Physics, Soongsil University, Seoul 156-743, Korea, G. CAO, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA — Recently, the effect of spin-orbit coupling in 5d transition metal oxides attracted lots of attention. It was found that the cooperative interaction of spin-orbit coupling and electron correlation could realize unique Mott insulating ground state of Sr$_2$IrO$_4$. We investigated temperature-dependent optical conductivity spectra of 5d Mott insulator Sr$_2$IrO$_4$. We observed drastic changes of the optical conductivity spectra. As temperature increases, the Mott gap was significantly reduced and spectral weight redistribution between the Ir $t_{2g}$ bands occurred. The electronic structure changes accompanied the change of optical phonon modes. These experimental observations could be understood in terms of the effects of spin-orbit and electron-lattice coupling.

10:24AM A30.00013 LS separation of J=1/2 Mott insulator observed by magnetic X-ray diffraction, SHIGEKI FUJIIYAMA, RIKEN, B.J. KIM, Univ, Tokyo, H. OHSUMI, T. KOMESU, SPRing-8, RIKEN, D. HIRAI, K. OHASHI, Univ, Tokyo, S. SAKAI, SPRing-8, RIKEN, T. ARIMA, Tohoku Univ., H. TAKAGI, Univ, Tokyo — Spin-orbit coupling is a key concept to realize spin Hall effect in insulating materials. A perovskite iridate Sr$_3$Ir$_2$O$_7$ shows a broad distribution of hyperfine fields implying a large distribution of local environments at Mn sites. The hyperfine distribution may be linked to orbital ordering effects. Mn spin – lattice relaxation rates have a surprisingly weak dependence both on temperature and applied magnetic field. Significant departures of the relaxation rate from Korringa temperature dependence below 20 K provide evidence for non-Fermi liquid behavior in this quasi-2D metal. At temperatures approaching $T_c$ from below, further anomalous behavior is found consistent with spin polaron formation in the range where colossal magnetoresistance starts to appear.

10:36AM A30.00014 Magnetization reversal in Sr$_3$Ir$_2$O$_7$: DM interactions vs. magnetic single-ion anisotropy. HOSUB JIN, JAEJUN YU, Department of Physics and Astronomy, Seoul National University — Recently the unusual insulating ground state of Sr$_3$Ir$_2$O$_7$ was shown to be a consequence of a novel quantum ground state of $J_{eff}$=1/2. Another compound in its series Sr$_3$Ir$_2$O$_7$ with double layers of the IrO$_2$ planes exhibits anomalous magnetic responses such as magnetization reversal during field-cooling processes. We performed density-functional theory calculations to investigate the electronic and magnetic properties of Sr$_3$Ir$_2$O$_7$. Similarly to the case of Sr$_3$Ir$_2$O$_7$, both spin-orbit (SO) and on-site Coulomb interactions are found to be responsible for the insulating ground state. Based on the analysis of our first-principle calculations for the various spin and lattice configurations, we found that the non-zero angular momentum state originating from large SO interactions with lattice distortions plays a crucial role in determination of both single-ion anisotropy and Dzyaloshinski-Moriya interactions, which explains anomalous magnetic responses in Sr$_3$Ir$_2$O$_7$. 
10:48AM A30.00015 Post-perovskite transition and magnetic and charge transport properties of the correlated 4d post-perovskite CaRhO₃ — K. YAMURA, Y. SHIRAKO, H. KOJITANI, M. ARAI, D.P. YOUNG, M. AKAOGI, M. NAKASHIMA, T. KATSUMATA, Y. INAGUMA, E. TAKAYAMA-MUROMACHI — A high-quality polycrystalline sample of the correlated 4d post-perovskite CaRhO₃ (Rhf+1.4d⁰ S = 1/2) was attained under a moderate pressure of 6 GPa for the first time. It is obvious that the perovskite CaRhO₃ transforms into a layered phase, in which Rh₃O₆ octahedra are connected by shearing the edge along a-axis and the corner along c-axis. The Rh-O layer stacks up alternatively with the Ca layer along b-axis. The characteristic structure suggests an electronic anisotropy toward 2D, which may be essential for unusual magnetism. The sample was subjected for measurements of charge transport and magnetic properties. The data clearly indicate it goes in an antiferromagnetically ordered state below ~90 K in an unusual way, being a strikingly contrast to what was observed for the perovskite phase.

Monday, March 16, 2009 8:00AM - 11:00AM –
Session A31 GMAG DMP: Focus Session: Molecular Nanomagnets 335

8:00AM A31.00001 Molecular Spintronics using Molecular Nanomagnets, WOLFGANG WERNSDORFER, CNRS, Institut Neel — A revolution in electronics is in view, with the contemporary evolution of two novel disciplines, spintronics and molecular electronics. A fundamental basis of these two fields can be established on magnetic molecules, and in particular, single-molecule magnets [1], which combine the classic macroscopic properties of a magnet with the quantum properties of a nanoscale entity. The resulting field, molecular spintronics aims at manipulating spins and charges in electronic devices containing one or more molecules. In this context, we want to fabricate, characterize and study molecular devices (molecular spin-transistor, molecular spin-valve and spin filter, molecular double-dot devices, carbon nanotube nano-SQUIDs, etc.) in order to read and manipulate the spin states of the molecule and to perform basic quantum operations. The talk will discuss this—still largely unexplored—field and present our first important results [2,3].


8:36AM A31.00002 Entrapment of magnetic micro-crystals for on-chip ESR studies, NICKOLAS GROLL, SYLVAIN BERTAINA, Department of Physics and National High Magnetic Field Laboratory, Florida State University, MEKHALA PATI, Department of Chemistry and Biochemistry, Florida State University, NARESH S. DALAL, Department of Chemistry and Biochemistry and National High Magnetic Field Laboratory, Florida State University, IRINEL CHIORESCU, Department of Physics and National High Magnetic Field Laboratory, Florida State University — On-chip Electronic Spin Resonance (ESR) of magnetic molecules requires the ability to precisely position nanosized samples in antinodes for a maximum magnetic coupling. A method is developed to entrap micro-crystals containing spins in a well-defined location on the substrate surface. Through the use of photolithography, this method has achieved positioning of single to tens of crystals with micron scale resolution. The method has allowed Q-band EPR measurements of a 175 micron diameter single crystal of BDPA at 34 GHz. Polycrystalline diluted Cr³⁺ spin 1/2 systems [1] have been entrapped in 500 micron squares for which the lower limit of the EPR measurement sensitivity was approached. This method gives way to on-chip ESR measurements at dilution refrigerator temperatures by allowing the samples to be positioned inside an on-chip superconducting cavity. [1] N. Sarita et al, Phys. Rev. Lett. 99, 137601 (2007).

8:48AM A31.00003 Experimental determination of the dipolar field in Mn₁₂-acetate₁, SEAN MCHUGH, R. JAAFAR, M.P. SARACHIK, City College of New York, Y. MYASOEDOV, H. SHTRIKMAN, E. ZELDOV, The Weizmann Institute of Science, R. BAGAI, G. CHRISTOU, University of Florida - Gainesville — Crystals of the molecular magnet Mn₁₂-acetate are known to contain a small fraction of defect (minor species) molecules with a small anisotropy barrier against spin reversal. The lower barrier leads to faster magnetic relaxation and lower coercive field. We exploit the low coercive fields of the minor species, and the location of the minor species tunneling resonances, to make a direct determination of the dipolar field in Mn₁₂-acetate. We find that the dipolar field of a fully magnetized crystal is 51.5 ± 8.5 mT, consistent with theoretical expectations.

1 Work at CCNY supported by NSF grant DMR-00451605.

9:00AM A31.00004 Magnetization barrier reduction in Mn₁₂ single-molecule magnets, GAGE REDLER, CHANGHYUN KOO, SAITI DATTA, Department of Physics, University of Florida, Gainesville, FL-32611, USA, CHRISTOS LAMPROPOULOS, THEOCARIS C. STAMATATOS, GEORGE CHRISTOU, Department of Chemistry, University of Florida, Gainesville, FL-32611, USA, STEPHEN HILL, Department of Physics, University of Florida, Gainesville, FL-32611, NHMF and Department of Physics, Florida State University, Tallahassee, FL-32310 — High-frequency electron paramagnetic resonance (HF-EPR) and AC susceptibility data will be presented for a new high-symmetry Mn₁₂-ac complex, [Mn₁₂O₁₂(R(OAc)₆)(MeOH)]₂⁻·MeOH, in which the acetic acid solvent is replaced by a single methanol. The results are compared with those of several other Mn₁₂ single-molecule magnets (SMMs), including Mn₁₂Ac²⁻·2CH₃COOH. AC susceptibility studies indicate that Mn₁₂Ac²⁻·MeOH has a relatively large effective barrier, Uₑff ~ 74 K, in comparison to Mn₁₂Ac²⁻·2CH₃COOH. Meanwhile, EPR studies suggest more-or-less identical zero-field-splitting parameters for the two complexes. Based on these findings, we discuss the factors that can lead to reductions in Uₑff in various Mn₁₂ SMMs.

9:12AM A31.00005 The role of quantum tunneling in magnetic avalanches in Mn₁₂-acetate₁, XIANG MA, BO WEN, S. MCHUGH, M.P. SARACHIK, City College of New York, Y. MYASOEDOV, H. SHTRIKMAN, E. ZELDOV, The Weizmann Institute of Science. R. BAGAI, G. CHRISTOU, University of Florida - Gainesville — Steps occur in the hysteresis loop of the molecular magnet, Mn₁₂-ac due to quantum tunneling at “resonant” magnetic fields where the energies of levels on opposite sides of the anisotropy barrier corresponding to different spin projections cross. The effect of quantum tunneling is also evident when magnetic relaxation occurs abruptly as a magnetic avalanche where spin reversal occurs along a narrow front that travels at subsonic speed. In particular, studies have shown that the ignition temperature displays minima and the velocity of the avalanche front shows maxima at the resonant fields. We report measurements of the avalanche speed triggered in an external magnetic field applied at an angle with respect the c-axis of the crystal, which the transverse component provides a symmetry-breaking field that increases the tunneling rate and magnetic relaxation.

1 Work at CCNY supported by NSF grant DMR-00451605.

9:24AM A31.00006 Tuning magnetization avalanches in Mn₁₂-acetate₁, BO WEN, S. MCHUGH, XIANG MA, M.P. SARACHIK, City College of New York, Y. MYASOEDOV, H. SHTRIKMAN, E. ZELDOV, The Weizmann Institute of Science, R. BAGAI, G. CHRISTOU, University of Florida - Gainesville — We report the results of a systematic study of magnetic avalanches (abrupt magnetization reversals) in the molecular magnet Mn₁₂-acetate using a micron-sized Hall sensor array. Measurements were taken for: (a) fixed magnetic field (constant barrier against spin reversal); and (b) fixed energy release obtained by adjusting the barrier and ∆M. A detailed comparison with the theory of magnetic deflagration of Garanin and Chudnovsky [1] will be presented and discussed. [1] D. A. Garanin and E. M. Chudnovsky, Phys. Rev. B 76, 054410 (2007).

1 Work at CCNY supported by NSF grant DMR-00451605.
9:36AM A31.00007 Non-adiabatic spin transition in the presence of phonon bottleneck effect, LEI CHEN, IRINEL CHIORESCU, Department of Physics and the National High Magnetic Field Laboratory, Florida State University — We present a study on deviations of the magnetization cycle of a two-level spin system from a reversible function into an opened hysteresis cycle due phonon bottleneck effect combined with Landau-Zener transitions. In the case of large zero-field level repulsion the magnetization curves can be described by a simple phonon-bottleneck model, in agreement with recent experiments on molecular magnets (V15 and Ru2) [1]. In the case of small tunneling gaps, as for large spin systems (Mn12 or Fe8), the spin will tunnel with a probability given by the Landau-Zener mechanism. The phonon-bottleneck model is here generalized into a model able to blend the non-adiabatic dynamics of spins with the presence of a non-equilibrium phonon bath [2]. Bloch equations are written in the eigenbasis of the effective spin Hamiltonian, assumed to be a two-level system at low temperatures, with a relaxation term driven by the phonon-bottleneck mechanism.


9:48AM A31.00008 Geometric-Phase Effect in the Thermally Assisted Resonant Tunneling of Mn12-tBuAc, J.R. FRIEDMAN, E. H. DA SILVA NETO, Amherst College Physics Dept., C. LAMPROPOULOS, G. CHRISTOU, University of Florida Chemistry Dept., N. AVR AHAM, Y. MYAESOE DOV, H. SHTRIKMAN, E. ZELDOV, Weizmann Institute of Science — Mn12-tBuAc, like the better-known single-molecule magnet Mn12-Ac, relaxes between up and down spin states by thermally assisted resonant tunneling when a longitudinal magnetic field (H_L) brings energy levels into resonance. In Mn12-Ac, tunneling is induced by a second-order transverse anisotropy produced by local solvent disorder. Such disorder makes the observation of any possible geometric-phase interference effect impractical. Mn12-tBuAc, in contrast, has negligible solvent disorder and an intrinsic fourth-order transverse anisotropy. We present experimental data on the transverse-field (H_T) dependence of the magnetic relaxation rate for Mn12-tBuAc. When on resonance (H_L = 0), the rate increases as a function of H_T in a series of steps and plateaus due to abrupt changes in the dominant tunneling pair of levels. Surprisingly, a similar effect occurs when off resonance (i.e. large H_L). Detailed numerical simulations show that the experimental results, both on and off of resonance, can be well described if the fourth-order anisotropy is included in the spin Hamiltonian. The results can be understood as arising from a geometric-phase effect that occurs when H_T is applied along the hard axis. Support: NSF grant #DMR-0449516.

10:00AM A31.00009 GGA+U study of exchange interactions in a Mn5 single-molecule magnet, EMAL E POPOFF, Virginia Tech, Blacksburg, VA, SALVADOR BARRAZA-LOPEZ, Georgia Tech, Atlanta, KYUNGWHA PARK, Virginia Tech, Blacksburg, VA, HUI-LIEN TSAI, Department of Chemistry, National Cheng Kung University, Taiwan — Electronic structure of a single-molecule magnet (SMM) Mn5 is investigated using GGA+U formalism. There are two types of Mn ions in the SMM Mn5: Mn3+ (S = 2) and Mn2+ (S = 5/2). In a prototype single-molecule magnet Mn12, superexchange interactions between Mn ions through oxygen anions are known to be antiferromagnetic. Our calculation on Mn5, however, showed that the Mn ions are all ferromagnetically coupled to each through various ligands. This results in the ground state spin of S = 11, which is in good agreement with experiment. We discuss the nature of the ferromagnetic coupling between the Mn ions by analyzing calculated projected density of states.

10:12AM A31.00010 ABSTRACT HAS BEEN MOVED TO SESSION S1 —

10:24AM A31.00011 Magnetism and magnetic anisotropies of small organic molecules, JAIME FERRER, DIEGO CARRASCAL, LUCAS FERNANDEZ SEIVANE, Universidad de Oviedo / CINN — The ability to enhance and tailor the magnetism of small atomic clusters and molecules will determine whether nanospintronics can be used as a storage technology. We present here our ab initio studies on the magnetism of small organic molecules containing transition metal atoms. We focus specially on 5d atoms like gold, platinum and iridium. These have a large spin-orbit interaction, which generates large magnetic anisotropies in small atomic clusters [1]. [1] L. Fernandez Seivane and J. Ferrer, Phys. Rev. Lett. 99, 183401 (2007).

1:00PM A32.00012 Anisotropic exchange in a tetranuclear CoIII complexes, SAITI DATTA, JUNJIE LIU, JON LAWRENCE, Department of Physics, University of Florida, Gainesville, FL 32611, CHRISTOPHER C. BEEDLE, DAVID N. HENDRICKSON, Department of Chemistry and Biochemistry, University of California at San Diego, La Jolla, CA 92093, STEPHEN HILL, Department of Physics, University of Florida, Gainesville, FL 32611, NHMFL and Department of Physics, FSU, Tallahassee, FL 32310 — High-frequency electron paramagnetic resonance (HFEPR) studies of the tetranuclear CoIII complex [Co(hmp)(dmb)Cl]+ reveal the presence of significant zero-field-splitting (ZFS) within the ground state spin multiplet. Meanwhile, low-temperature hysteresis measurements of 1 provide evidence for slow magnetization relaxation, suggesting that it could be a single-molecule magnet (SMM). However, HFEPR studies of a Zn analog of 1, doped with a small quantity of CoII, show the ground state of the CoII ions to be an effective spin S′ = 1/2 Kramers doublet with a highly anisotropic g-tensor. To understand the origin of the ZFS within the ground state spin multiplet of 1, as well as the slow magnetization relaxation, we consider the effect of anisotropic and antisymmetric exchange interactions between the ions within the tetranuclear complex. Our model provides an explanation for the ZFS in the ground state observed via HFEPR, and can also account for qualitative features observed through magnetic measurements.

10:48AM A31.00013 Magnetization studies of a new single molecule magnet [Net4][Mn3Zn2(salox)3O(N3)6Br2], JOHN HENDERSON, ENRIQUE DEL BARCO, University of Central Florida, CHANGHYUN KOO, STEPHEN HILL, Florida State University/NHMFL, PATRICK FENG, DAVID HENDRICKSON, University of California at San Diego, MOTOHIRO NAKANO, Osaka University — We present magnetization studies of a novel S = 6 single molecule magnet (SMM) [Net4][Mn3Zn2(salox)3O(N3)6Br2] (Mn3). The results reveal extremely clean changes in the magnetization associated to the high crystalline quality of the compound. The sample allows a detailed study of the role of molecular symmetry on the nature of the magnetic quantum tunneling relaxation of these molecules. Experiments at temperatures down to 30 mK carried out in a 3D vector superconducting magnet will be presented. The possible role of phonons as originators of the tunneling relaxation of the magnetization in this SMM will be used to explain interesting experimental observations.

Monday, March 16, 2009 8:00AM - 11:00AM —
Session A32 GMAG: Magnetization and Spin Dynamics 336
8:00AM A32.00001 Nanomagnetic Spin Fluids1, SKOMSKI RALPH, University of Nebraska, A. ENDERS, R. D. KIRBY, D. J. SELLMYER — The dynamics of conventional magnets is governed by the static micromagnetic response to an external magnetic field, with corrections due to thermal excitations. For example, permanent magnets undergo aging (magnetic viscosity), and magnetic recording media lose some of the stored bits due to thermal excitation. Essential deviations from this Arrhenius (or Néel- Brown) behavior occur on a length scale below about 2 nm. The relaxation no longer obeys Kramer's escape-rate theory and must be replaced by path-integral considerations with nontrivial activation-energy contributions. This presentation investigates several theoretical and experimental aspects of unusual magnetization dynamics in small-scale wires, thin films and dots. The first explicit example is the formation of liquid-like droplets, observed in ultrathin films with perpendicular magnetic anisotropy and characterized by 180° domains of well-defined chirality. (The one-dimensional equivalent of this phenomenon is a hard-core gas with particle-number conservation.) The second example is of theoretical nature and links the phenomenon of slow magnetization dynamics to the concept of fractional kinetics. A general feature of the considered nanomagnets is their resemblance to fluids (liquids or gases), as opposed to the glassy dynamics of conventional magnets.

1This work is supported by NSF MRSEC and NCMN.

8:12AM A32.00002 Interface Magnetization Switching and Demagnetization in Fe/Al films and Fe/Pt nanoparticles, WEI LAI, TETIANA NOSACH, YU GONG, YUHANG REN, CHAEHYUN KIM, SAVAS DELIKANL1, HAO ZENG, THE ULTRAFAST OPTICS GROUP AT HUNTER COLLEGE OF THE CITY UNIVERSITY OF NEW YORK TEAM, SPIN EFFECTS AND NANOMAGNETISM GROUP AT THE UNIVERSITY AT BUFFALO TEAM — We report on the reversal and demagnetization processes of the Fe interface layer magnetization in thin films and nanoparticles of Fe/Al and Fe/Pt by time-resolved magnetization-induced second-harmonic generation. The results are compared with those of the bulk magnetization as obtained from magneto-optic Kerr effect. We realize that switching and demagnetization characteristics are distinctly different between bulk and interface layers because of the interface-derived anisotropy and the dipole interactions. In particular, the surface and interface magnetism will dominate the behaviors of nanoscale structures.

8:24AM A32.00003 Magnetization hysteresis studies in Sm1-xGd12Al2 alloys, U. VAIYDA, S. VENKATESH, V.C. RAKHECHA, DCMP&MS, Tata Institute of Fundamental Research, Mumbai, India, S. RÁMAKRISHNAN, A.K. GROVER, DCMP&MS, Tata Institute of Fundamental Research, Mumbai, India — SmAl2 (Tc ~ 125 K, μsat = 0.23 μB/f.u.) is known to exhibit magnetic compensation when doped with Gd (0 < x < 0.5). In such stoichiometries though the magnetization gets closer to zero, there exists a large spin polarization. This makes such materials attractive candidates for applications. We have performed detailed magnetization hysteresis and other studies in the series Sm1-xGd12Al2. In x=0.02 alloy, the loops are shifted (notion of exchange bias) along negative H-axis for temperatures just above Tcomp and along positive H-axis for temperatures T > Tcomp. We argue that the change in the sign of exchange bias is due to the magnetic contribution of conduction electron polarization as well as that of local magnetic moments reversing the signs. At Tcomp, the width of the hysteresis loop collapses. In the given series, one can set up the system in either spin-surplus or orbital-surplus state and control the exchange bias field. The compositions with 0.03 < x < 0.06 do not exhibit zero cross over of magnetization and remain spin surplus. Our various studies and analysis shall be presented.

8:36AM A32.00004 New spin modes in itinerant ferromagnets, JOHN FELDMANN, KEVIN BEDELL, Boston College — We are theoretically investigating new collective spin phenomena that could exist in itinerant ferromagnetic materials such as MnSi. We postulate an attractive candidate for applications. We have performed detailed magnetization hysteresis and other studies in the series Sm1-xGd12Al2. In x=0.02 alloy, the loops are shifted (notion of exchange bias) along negative H-axis for temperatures just above Tcomp and along positive H-axis for temperatures T < Tcomp. We argue that the change in the sign of exchange bias is due to the magnetic contribution of conduction electron polarization as well as that of local magnetic moments reversing the signs. At Tcomp, the width of the hysteresis loop collapses. In the given series, one can set up the system in either spin-surplus or orbital-surplus state and control the exchange bias field. The compositions with 0.03 < x < 0.06 do not exhibit zero cross over of magnetization and remain spin surplus. Our various studies and analysis shall be presented.

8:48AM A32.00005 Scaling collapse of the irreversible magnetization of ferromagnetic thin films1, R. DAS, A.F. HEBARD, University of Florida, Department of Physics — The irreversible magnetization, ΔM, defined as the difference of field-cooled magnetization MFC and zero-field-cooled magnetization MZFC, has been measured for a variety of ferromagnetic thin films as a function of magnetic field H at different temperatures T. Isotherms of ΔM show maxima ΔMmax at characteristic temperature-dependent fields Hm(T) at very low and high magnetic fields the values of MFC and MZFC converge and ΔM is observed to approach zero in these limits. If ΔM/ΔMmax is plotted as a function of H/Hm for a given ferromagnetic system, the graphs for different temperatures collapse onto the same curve. This scaling collapse is clearly seen for three different ferromagnetic thin-film systems: polycrystalline gadolinium, phase separated manganites, and single domain Ni nanomagnetic grains embedded in an insulating host. Similar scaling behavior has also been observed in spin-glass material [1]. These results represent a heretofore unrecognized scaling behavior that appears to apply to a broad range of ferromagnetic systems. [1] V. S. Zotev, G. G. Kenning, and R. Orbach, Phys. Rev. B 66, 014412 (2006)

1Work supported by NSF grant #DMR-0704240.

9:00AM A32.00006 Atomic spin-dynamics simulations from first principles theory, OLLE ERIKSSON, Upssala University — In this talk I will present recent developments in atomic spin-dynamics simulations using first principles theory. Details of the implementation will be given and simulations of spin-glass materials (Cu-Mn) and diluted magnetic semiconductors (Mn doped GaAs) will be presented.

9:12AM A32.00007 Dynamics of Einstein - de Haas Effect: Application to Magnetic Cantilever, REEM JAAFAF, E.M. CHUDNOVSKY, D.A. GARANIN, Lehman College, The City University of New York — Local time dependent theory of Einstein - de Haas effect is developed. We show that internal elastic twists that accompany dynamics of spins enter equations of elasticity in the universal form that does not require precise knowledge of spin-lattice interactions. As long as the space-time dependence of the magnetization is known, local elastic deformations can be computed rigorously without any unknown parameters. The theory is applied to the description of the motion of a magnetic cantilever caused by the oscillation of the domain wall. Theoretical results are compared with a recent experiment on Einstein - de Haas effect in a microcantilever.

9:24AM A32.00008 Colored thermal noise in spin valves, JIANG XIAO, GERRIT BAUER, Kavli Institute of NanoScience, Delft University of Technology, Delft, The Netherlands, SADAMICHI MAEKAWA, Institute for Materials Research, Tohoku University, Sendai, Japan, ARNE BRATAAS, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway — We report a theoretical study of the thermal electrical noise in spin valves. There are two independent noise sources in spin valves: 1) thermal agitation of charge carriers causing Johnson-Nyquist noise, 2) thermal agitation of the magnetization that contributes to the electric noise by spin and charge pumping. The noise power spectrum from the latter consists of two absorption lines at zero frequency and at the ferromagnetic resonance on top of a white noise background. The relative intensities depend on the magnetization configuration.
9:36AM A32.00009 Numerical evidence for unstable magnons at high fields in the square lattice Heisenberg antiferromagnet, OLAV F. SYLJUÅSEN, Department of Physics, University of Oslo — We have found numerical evidence for decaying magnons in the square lattice spin-1/2 Heisenberg antiferromagnet when it is exposed to a strong external magnetic field. The results are obtained using Quantum Monte Carlo simulations combined with a Bayesian inference technique to obtain dynamics, and are consistent with earlier predictions from spin wave theory.

9:48AM A32.00010 Low-Frequency Magnetization Noise in Spin-Valve Structures1, ARIF OZBAY, AISHA GOKCE, EDMUND NOWAK, THOMAS FLANAGAN, RYAN STEARRETT, University of Delaware, CATHY NORDMAN, NVE Corp. — We report on 1/f resistance noise due to thermally driven fluctuations of the domain structure in GMR and MTJ sensors. Resistance noise from both the free layer (FL) and reference layer (RL) is evident. A near linear scaling of the normalized noise power with the sensor’s sensitivity is observed. For a given sensitivity, the RL exhibits higher noise than the FL. This appears correlated to the larger imaginary (dissipative) component in the resistance susceptibility of the RL. In addition, we find that the imaginary component is larger for layers that exhibit pronounced magnetic hysteresis, suggestive of connection between the noise and relaxation processes. A model based on equilibrium magnetization fluctuations is in good quantitative agreement with the measured noise power over most of the sensor's borengiasis response. A magnetic 1/f noise parameter is defined which can be used to compare magnetoresistive sensors having differing sizes, sensitivities, and under different biasing conditions.

1DOE and Office of Naval Research

10:00AM A32.00011 Phase Diagram of Equilibrium Domain-Wall Solutions in Finite-Size ECC Media, SONALI MUKHERJEE, Seagate Technology, LUC BERGER, Carnegie Mellon University — Reversal in ECC media where hard and soft anisotropy magnetic material are exchange coupled has been studied because it has high thermal stability with low reversal field. Using Euler-Lagrange condition, we have studied the field evolution of domain-wall solutions in ECC for various anisotropy ratios of hard and soft phase and soft-phase length scales. We find that there exist 3 critical fields. At the field H1, the domain-wall solution Es (surface domain-wall) and E1 (soft-phase domain-wall) start existing. The nucleation field Hn is the field where the energy of Es and the unreversed uniform solution E0 coincide. Above Hn, Es ceases to exist. The domain-wall propagation field Hdw is the field where the energy of soft domain-wall exist E1 and hard domain-wall E2 coincide. Above Hdw, E1 and E2 cease to exist. The reversal field is the field at which no domain-wall solutions exist anymore and is the maximum of Hn and Hdw fields. The field Hn is found to reduce with increasing soft-phase length, and Hdw is found to be independent of the phase ratio greater than the higher wall width of the hard phase. For hard/soft anisotropy ratio kh/kS less than 5, the nucleation field is always dominant. When kh/kS is greater than 5, there exits a soft-phase length lsc, at which the fields Hn and Hdw become equal and is greater than lsc. Hdw dominates the reversal and, when lsc is smaller than lsc, Hn is the reversal field.

10:12AM A32.00012 Nature of magnetic ordering in Ni(OH)2 nanoplates, JAMES RALL, MOHANDIR SEEHRA, West Virginia University — Nickel hydroxides are important for their potential applications in rechargeable batteries and as precursors for NiO and Ni catalysts. kappa-Ni(OH)2 has the CdCl2 layered structure with Ni atoms forming a hexagonal unit cell. Here, we report on the magnetic ordering in 17 nm x 4 nm nanosheets of Ni(OH)2. Measurements of the magnetization M as a function of temperature (2K to 300K) and magnetic field H up to ±55kOe are reported. M vs. T data in H=100 Oe for the ZFC case shows a peak in M at T = 24 K characteristic of antiferromagnetic (AF) ordering; however for T > Tc, the Curie-Weiss (χ = C/(T - θ)) fit yields θ = 26K characteristic of ferromagnetism. Following Takada (J. Phys. Soc. Jpn. 21, 274S, 1966), we measured M vs. H loops from T = 2K to 25K and observed a metamagnetic transition at Hc = 56 kOe at 2K, with Hc decreasing with increasing T. These results suggests strong ferromagnetic coupling among Ni within (001) sheets and a weaker antiferromagnetic coupling in the neighboring (001) sheets, and [001] as the easy axis. This model is used to determine the exchange constants consistent with the observed Curie-Weiss variation.

10:24AM A32.00013 First-principles calculations of laser-induced spin manipulation in small magnetic clusters with CO, CHUN LI, GEORGIOS LEFKIDIS, WOLFGANG HÜBNER, Kaiserslautern University of Technology — We present a fully ab initio controlled ultrafast magnetooptical switch and transfer mechanism in small magnetic clusters exploiting spin-orbit-coupling enabled Lambda-processes [1-3]. Two-magnetic-center clusters with CO attached to one of the magnetic atoms are studied to achieve a mapping of the laser-induced spin manipulation to the IR spectrum of CO. The predicted spin-state-dependent CO frequencies can facilitate experimental monitoring of the processes. The lower electronic states of the clusters exhibit a very high degree of spin localization either at the Co or the Ni site. Spin flip on one magnetic atom and transfer from one magnetic center to the other are realized in structurally optimized magnetic clusters with fidelities that reach 99.8%. Electron states of the clusters exhibit a very high degree of spin localization either at the Co or the Ni site. Spin flip on one magnetic atom and transfer from one magnetic center to the other are realized in structurally optimized magnetic clusters with fidelities that reach 99.8%.


10:36AM A32.00014 Magnetic properties of a doped quasi-triangular lattice material, Cu2(1−x)Zn2x(9OH)2NO3/(C17H15COO), JIAN WU, ANUP K. GANGOPADHYAY, S.A. SOLIN, Washington University in St. Louis — Cu2(OH)2NO3 is a geometrically frustrated layered compound in which spin S=1/2 Cu2+ ions are arranged on a slightly distorted triangular lattice. The magnetic properties of the pure compound and of the compound intercalated with alkane carboxylate have been extensively studied.[1] However, the effects of interlayer doping remain unexplored. The substitution of non-magnetic ions such as Zn2+ for Cu2+ will ultimately drive the ordering temperature toward zero[2] which may provide a candidate system possessing an exotic spin-liquid ground state. We have prepared powder samples of the Cu2(1−x)Zn2x(9OH)2NO3 family and systematically investigated them by magnetic susceptibility measurements. The ordering temperature decreases from 11K to 5.6K while the Cu-W temperature increases from -5.1K to +2.8K as the Zn concentration increases from 0 to 65%. To enhance the 2-dimensional characteristic and reduce the interlayer interaction, we introduce an alkanecarboxylate C7H15COO- into the interlayer space. The experimental results we have obtained indicate that this new class of materials have much higher frustration levels [θ2ω / Tc] ~ 20 and order at a lower temperature than the doped parent compounds.


10:48AM A32.00015 Coupling between optically-induced coherent spin and lattice dynamics in epitaxial Fe films, VLADIMIR STOICA, University of Michigan, DON WALKO, Argonne National Laboratory, ERIC LANDAHL, DePaul University, YUELIN LI, Argonne National Laboratory. ROY CLARKE, University of Michigan — Spin dynamics excitation using femtosecond optical pulses in ferromagnetic thin films is a powerful technique to study spin dependent interactions in solids. One topic of interest is the temporal separation of relaxation processes related to fundamental interaction mechanisms, which include spin-orbit, spin-lattice and exchange coupling. Establishing experimentally the relaxation timescales for these couplings is an important step that assists the development of new spintronic applications. We employ time-resolved magneto-optical and X-ray diffraction probes to separate spin and lattice interactions in epitaxial Fe films grown by molecular beam epitaxy on Ge and MgO substrates. We study the connection between the magnetic and lattice relaxation times excited by optical pulses. We find that coherent spin precession dynamics correlates well with thermoelastic strain relaxation from picosecond to nanosecond time scales.
8:00AM A33.00001 Temperature dependent ARPES study of the pseudogap of Pb-Bi2201.

MAKOTO HASHIMOTO, RUHUA HE, Stanford, KIYOHISA TANAKA, JEAN-PIERRE TESTAUD, Stanford/LBL, WORAWAT MEEVASANA, ROB MOORE, DONGHUI LU, Stanford, YOSHIYUKI YOSHIDA, HIROSHI EIASKI, AIST, ZAHID HUSSAIN, LBL, ZHI-XUN SHEN, Stanford — The pseudogap phenomena in the high-Tc cuprates have been extensively studied because of possible intimate connection with the unknown mechanism of superconductivity. We have studied the ARPES spectra of optimally-doped Pb-Bi2201 (Tc = 34 K) at SSRL BL5-4, from the superconducting state (10 K) to the normal state above the pseudogap temperature (160 K). We have revealed how the band structure changes with the pseudogap opening, and found that the superconducting gap alone cannot explain the ARPES spectra in the antinodal region. Based on the results, in the presentation, we would like to discuss possible origins of the pseudogap. This work is supported by the DOE Office of Basic Energy Science, Division of Materials Science and Engineering. ARPES experiments were performed at the Stanford Synchrotron Radiation Laboratory (SSRL), which is operated by the Department of Energy Office of Basic Energy Science.

8:12AM A33.00002 Pseudo-gap in electron doped cuprates: Spin fluctuation origin and close relation with superconducting gap. SEUNG RYONG PARK, Yonsei university, Korea, D.J. SONG, C.S. LEEM, CHUL KIM, S.K. CHOI, Y.K. KIM, C. KIM, K.J. CHOI, J.H. KIM, Yonsei University, K.M. SONG, Inha University, Korea, JUNG HOON HAN, Sungkyunkwan, Korea, Y. YOSHIDA, H. EIASKI, AIST, Japan — A natural candidate for the cause of PG in electron doped cuprates could be spin fluctuations. However, there has not been any careful calculation based on the spin fluctuation model, at least to our best knowledge. Recently, dynamic spin susceptibility measurement on electron doped cuprates was obtained by using inelastic neutron scattering. Therefore, one could use electron-spin coupling which is proportional to the dynamic spin susceptibility and calculate the spectral function based on the electron-spin fluctuation coupling model. In this presentation, we first show calculated ARPES spectral function based on electron-spin fluctuation coupling model with the magnetic susceptibility as the input. We could identify the origin of PG as electron-spin fluctuation from this simulation, and we also could extract a rough value for the electron-spin fluctuation coupling strength g in electron doped cuprates by comparison between experimental data and simulation results.

8:24AM A33.00003 Temperature dependent ARPES study of the superconducting gap in overdoped Bi22121. H.-B. YANG, CMPMSD, Brookhaven National Laboratory, J.D. RAMEAU, CMPMSD, Brookhaven National Laboratory/ Stonybrook University, G.D. GU, P.D. JOHNSON, CMPMSD, Brookhaven National Laboratory — High-resolution angle-resolved photoemission (ARPES) is used to probe the temperature dependence of the superconducting gap around the Fermi surface in overdoped Bi2212. Lucy-Richardson deconvolution is applied to reduce the error from experimental resolution. Normalizing by the Fermi function then allows the observation of the true gap in the spectral function. Numerical simulation is also used to compare the experimental results with theoretical models. We have investigated the temperature dependence of the gap around the nodal region and the anti-nodal region, with temperature going from the superconducting state to the normal state.

1This work is supported by the Department of Energy under Contract No. DE-AC02-98CH10886

8:36AM A33.00004 ABSTRACT WITHDRAWN —

8:48AM A33.00005 ARPES study of YBa2Cu3O7−δ from the over to the underdoped regime by in situ K evaporation. G. LEVY, DAVID FOURNIER, M.A. HOSSAIN, J.D.F. MOITERSHEAD, UBC, J.L. MCHECHEYNE, A. BOSTWICK, E. ROTENBERG, ALS, W.N. HARDY, R. LIANG, C.A. SAWATZKY, I.S. ELFIMOV, D.A. BONN, A. DAMASCHELLI, UBC — Unravelling the nature of the electronic excitations in the underdoped regime of the Cuprates is a key element for understanding the fundamental mechanism behind HTSC. The YBCO phase diagram has been studied with photoelectron spectroscopy (ARPES) using a new in situ electron doping approach based on controlled potassium deposition [1] onto as-cleaved samples. All of the compounds studied (δ=0.5,0.66) exhibit heavily over-doped nature with well defined LDA-like Fermi surfaces and evolve toward disconnected Fermi arcs in the underdoped regime. These results are consistent with previous ARPES measurement on the HTSCs and in contrast with the quantum oscillations observations [2].


9:00AM A33.00006 Quasiparticles in Bi22121. M. VISHIK, W.-S. LEE, Stanford University, K. TANAKA, Osaka University, B. MORITZ, E.A. NOWADNICK, Stanford University, T. SASAGAWA, Tokyo Institute of Technology, T. FUJII, Tokyo University, T.P. DEVEREAUX, Z.-X. SHEN, Stanford University — From ARPES measurements, much has been learned about the single-particle excitations of the high-Tc cuprate superconductors, and collective properties can be inferred from these experiments too. The gap in the spectrum below Tc is related to the superconducting gap, and the superfluid density, the other hallmark of superconductivity, has been demonstrated to correlate closely with the weight of the antinodal quasiparticle peak. The momentum, temperature, and doping dependence of quasiparticle lifetime yields information about scattering processes, which are related to ground state properties. In Bi-2212 quasiparticles are present on the entire Fermi surface over a wide doping range. We present ARPES studies of the quasiparticles in Bi-2212 as a function of doping, momentum, and temperature, and discuss connections to other experiments.

9:12AM A33.00007 ARPES study on Tl-based Cuprates, WEI-SHENG LEE, KIYOHISA TANAKA, Stanford University & SIMES, SLAC, INNA VISHIK, Stanford University, DONGHUI LU, ROB MOORE, Stanford University & SSRL, SLAC, HIROSHI EIASKI, AKIRA IYO, AIST, Japan, THOMAS DEVEREAUX, ZHU-XUN SHEN, Stanford University & SIMES, SLAC — Here we report the angle-resolved photoemission measurements on nearly optimally multi-layer Tl-based superconducting copper oxides, including Tl2Ba2CaCu2O8 (Tl2212), Tl2Ba2Ca2Cu3O9 (Tl1223), and a comparison to the data of single layer Tl2Ba2CaCu2O8 (Tl-2212). Consistent with other optimally-doped cuprates, a hole-like Fermi surface and sharp quasi-particle peak in the superconducting state is observed. The renormalization effect due to the coupling of bosonic modes is also observed, which exhibits intriguing materials dependence. Implications of the observed material dependent renormalization effect will also be discussed.

9:24AM A33.00008 Anomalous behavior of the nodal scattering rate of Bi2Sr2CaCu2O8+δ near the Fermi energy, THEODORE REBER, NICK PLUMB, University of Colorado, JOHN DOUGLAS, NIST-Boulder, ZHE SUN, QIANG WANG, University of Colorado, YOSHIIRO AIURA, HIROSHI EIASKI, HIDEKI IWASAWA, AIST, MICHEL HERMELE, DANIEL DESSAU, University of Colorado — The scattering rate as determined by the width of a band is a direct measure of the imaginary part of a particle’s self-energy. Though the dispersion of a band can also used to extract the particle’s self-energy, the scattering rate is superior, because the ambiguity due to determining the underlying bare band is not included. The excellent momentum and energy resolution of low photon energy ARPES allows us to study the scattering rate of Bi2Sr2CaCu2O8+δ near the Fermi energy. Our studies show an anomalous feature that warrants continued study.
9:36AM A33.00009 Novel feature in the nodal electron self-energy and strong temperature dependence of the Fermi velocity in the high temperature superconductor Bi2212. N. C. PLUMB, T. J. REBER, University of Colorado, J.D. KORALEK, LBNL and UC Berkeley, Z. SUN, J. F. DOUGLAS, University of Colorado, Y. AIURA, K. OKA, H. EISAIK, AIST Tsukuba, D. S. DESSAU, University of Colorado — Using low-photon energy angle-resolved photoemission (ARPES), we study the low-energy dispersion along the superconducting node in Bi2212 as a function of temperature. Less than 10 meV below the Fermi energy, the high-resolution data reveals a novel "kink"-like feature in the real part of the electron self-energy. The kink is strongest below the superconducting critical temperature and appears to vanish as the temperature is raised. A corollary of this finding is that the Fermi velocity, as measured over this small energy range, varies rapidly with temperature — increasing by approximately 35% from 50 to 200 K. This is in contrast to the slope of the dispersion at only slightly deeper energy, which changes little by comparison and whose behavior is ostensibly dominated by the well-known 70-meV kink. We discuss some possible physical origins of the new low-energy feature, including the possibility that it may arise from bosonic mode couplings and/or nonanalytic corrections to Fermi liquid theory in 2D.

9:48AM A33.00010 ARPES investigation of two leg ladder compounds Sr14−xCaxCu24O41. GEY-HONG GWEEN, UC Santa Cruz, TAKAO SASAGAWA, Tokyo Institute of Technology. TAKAMI TOHYAMA, Yokawa Institute for Theoretical Physics, MATTHEW BRUNNER, JAMES HINTON, JACOB STANLEY, UC Santa Cruz — The so-called "two leg ladder compounds" Sr14−xCaxCu24O41 are interesting since it is well accepted that they form a resonating valence bond state. The crystal structure of two leg ladder compounds consists of one-dimensional motifs (ladders and chains), and it is within the ladders that the resonating valence bond state arises. As x is varied, these compounds go through a metal-insulator transition, and become a superconductor, albeit under pressure. So far, a high resolution ARPES study shedding light on the near-Fermi-level electronic structure of these interesting compounds has been missing. Here, we report our ARPES results, providing the first view of the near-Fermi-level quasi-one-dimensional electronic structure arising from the ladders. We discuss line shape features that are indicative of strong electron correlations.

10:00AM A33.00011 ARPES matrix element and the waterfall effect in the cuprates. SUSMITA BASAK, TANMOY DAS, Northeastern U., JOUKO NIEMINK, MATTI LINDOOES, Tampere U. Tech., Finland and Northeastern U., HSIN LIN, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern U. — The high-energy kink (HEK) or the 'waterfall' effect as seen in angle-resolved photoemission spectra (ARPES) in the cuprates has the potential of revealing important information about the dressing of quasiparticles by electronic excitations [1,2,3]. However, recently it has been suggested that matrix element effects are crucial in explaining the experimental spectra in Bi2Sr2CaCu2O8+δ (Bi2212), and it has been questioned whether the HEK exists [4]. Here we discuss how the interplay between the matrix element and self-energy effects shapes the ARPES spectra. Both the ARPES matrix element and the self-energy are found to be necessary for understanding the experimental spectra. Work supported in part by the USDOE. [1] R. S. Markiewicz et al., Phys. Rev. B 76, 174514 (2007). [2] A. Macridin et al., Phys. Rev. Lett. 99, 237001 (2007). [3] Tanmoy Das et al., cond-mat:0807.4257. [4] D.S. Inosov et al., Phys. Rev. Lett. 99, 237002 (2007).

10:12AM A33.00012 ABSTRACT WITHDRAWN

10:24AM A33.00013 LASER ARPES studies on Sr2RuO4. CHULIM SEUNG, SEUNG-PYONG KANG, C.S. LEEM, D.J. SONG, Y.K. KIM, S.K. CHOI, W.S. JUNG, Y.Y. KO, C. KIM, Institute of Physics and applied physics, Yonsei University, INSTITUTE OF PHYSICS AND APPLIED PHYSICS, YONSEI UNIVERSITY TEAM — LASER ARPES was performed on Sr2RuO4. With advance of LASER ARPES, we could perform bulk sensitive ARPES with 1meV energy resolution. With these advantages, intensive studies on Sr2RuO4 enlightened us more knowledge on layered structures.

10:36AM A33.00014 Fermiological interpretation for collective spin and charge orderings in underdoped La-based cuprates by ARPES. RUIHUA HE, Physics, Applied Physics, Stanford Univ. & SSRL (Stanford), KIYOHISA TANAKA, Stanford & ALS & Physics, Osaka Univ., SÜNG-KWAN MO, Stanford & ALS, HONG YAO, Stanford, MAKOTO Hishimoto, Stanford & ALS, EREZ BERG, Stanford, TAKAO SASAGAWA, Stanford & Materials and Structures Lab, TIT, TADASHI ADACHI, Applied Physics, Tohoku Univ., MASAKI FUJITA, Institute of Materials Research, Tohoku Univ., TEPEEI YOSHIDA, Complexity Science and Engineering, University of Tokyo, NORMAN MANNE, Stanford & ALS, WORAWAT MEESAVANAN, Stanford, YOJI KOIKE, Applied Physics, Tohoku Univ., KAZUYOSHI YAMADA, Institute of Materials Research, Tohoku Univ., ATSUHI FUJIMORI, Complexity Science and Engineering, University of Tokyo, STEVE KIVELSON, Stanford, ZAHID HUSSAIN, ALS, ZHI-XUN SHEN, Stanford — By using ARPES interpretation for the origin of the collective spin and charge orderings in underdoped La-based cuprate superconductors is carefully examined. A Fermi surface nesting wave vectors is identified which matches the collective ordering wave vector observed by neutron scattering for doping around 1/8. The pseudogap state is found to be essential for the development of such nesting instability of the electronic system toward density wave formation. A systematic doping dependence study will be presented that allows further insights into this issue.

10:48AM A33.00015 Mott gap collapse in the cuprates – apparent or real? . R. S. MARKIEWICZ, TANMOY DAS, A. BANSIL, Northeastern University — We have recently introduced a model self-energy for the cuprates, which includes an antiferromagnetic (AFM) transition dressed by spin and charge fluctuations.[1] This model correctly reproduces many 'strong coupling' features in the angle-resolved photoemission (ARPES) and optical spectra, including the waterfall effect and the doping dependence of the optical Mott gap. Here we discuss a dichotomy between Slater and Mott physics in the cuprates, with a Slater-like AFM gap collapse with doping in the coherent bands while the Mott-like gap persists in the incoherent bands. By analyzing the spectral weights, we show that there is an anomalous spectral weight transfer which is rather large to be consistent with strong coupling physics, but which is reasonably described by our intermediate coupling model. Work supported in part by the USDOE. [1] Tanmoy Das, R. S. Markiewicz, and A. Bansil, arXiv:0807.4257.

Monday, March 16, 2009 8:00AM - 11:00AM

Session A34 DCMP: Superconductivity: Spin Properties 404

8:00AM A34.00001 Evidence for Local Moment Magnetism in Superconducting Bi2Sr2CaCu2O8+δ. JOHN TRANQUADA, G.Y. XU, G.D. GU, M. HUECKER, Brookhaven Natl. Lab., B. FAUQUE, LLB, T.G. PERRING, C. STOCK, ISIS, L.-P. REGNAULT, CEA-Grenoble — We have used inelastic neutron scattering to measure the dynamic spin susceptibility in optimally-doped Bi2Sr2CaCu2O8+δ (Tc = 91 K). Four crystals with a total mass of 19 g were measured on the MAPS spectrometer at ISIS for temperatures of 10 K and 100 K. We have been able to identify the magnetic excitations in the energy range 20-90 meV. The magnetic nature of the scattering has been confirmed with spin-polarization analysis on IN22 at the ILL. While we see temperature-dependent changes for energies around 40 meV that are consistent with earlier studies, we find that the Q-integrated signal shows a much weaker variation with temperature. The absolute magnetic cross section is quite comparable to that of spin fluctuations in stripe ordered La2-xSr2xCuO4. As the magnetism in the latter system has been shown to have a dominant contribution from local moments [1], we argue that the same must be true for Bi2Sr2CaCu2O8+δ. [1] M. Huecker et al., Phys. Rev. B (accepted); cond-mat/0503417v3.

1Supported by Office of Science, US DOE, under Contract No. DE-AC02-98CH10886.
8:12AM A34.00002 Phase Separation and Magnetism in High Temperature Superconductors, S. WEN, Z. J. XU, G. D. GU, J. M. TRANQUADA, Brookhaven National Laboratory, M. V. ZIMMERMANN, HASYLAB at DESY, Hamburg, Germany — The pronounced stability of the charge and spin stripe order in La_{2-x}Sr_xCuO_4 at x = 1/8 doping still is a poorly understood peculiarity. A combination of electronic and structural interactions is likely, however it has been difficult to clearly separate the involved mechanisms. One approach is to explore how stripe order fades away for dopings x ≠ 1/8. We have performed high energy (100 keV) x-ray diffraction and static magnetization experiments on single crystals with x=0.095 and 0.155. To our surprise, at ambient pressure stripes exist in a much broader range of doping around x = 1/8 than expected. In the underdoped region charge stripe order always coincides with a structural transition associated with a rotation of the octahedral tilt axis. However, for x = 1/8 and high pressure we have been able to show that stripe order also occurs in the absence of this structural phase, which motivates us to discuss stripes in terms of an electronic liquid crystal phase.

1Supported by the US-DOE through contract DE-FG02-00ER45801.

8:24AM A34.00003 Stripe order in La_{2-x}Ba_xCuO_4 at ambient and high pressure, M. HUECKER, J. S. WEN, Z. J. XU, Department of Physics and Astronomy, McMaster University, T. ITO, P. L. RUSSO, A. T. SAVICI, Y. J. UEMURA, Department of Physics, Columbia University, H. KIM, S. WAKIMOTO, R. J. BIRGENEAU, Department of Physics, University of Toronto — There is now a large body of evidence from local probes which point to intrinsic heterogeneity in the cuprates. One example is the recent reports of an inhomogenous magnetic field response in the underdoped materials, as revealed by muon spin rotation experiments. In an effort to explore this field response, we have measured the /mu/0SR spectra of La_{2-x}Sr_xCuO_4 in a number of applied magnetic fields and with x ranging from the underdoped to heavily overdoped materials. I will summarize these efforts, and present the resultant data in the context of existing literature. Possible interpretations and directions for future research will be discussed.

8:36AM A34.00004 The local magnetic field response of La_{2-x}Sr_xCuO_4 on the overdoped side of the phase diagram as revealed by /mu/0SR, G. J. MACDOUGALL, Oak Ridge National Labs, A. A. ACZEL, S.-J. KIM, J. A. RODRIGUEZ, C. R. WIEBE, G. M. LUKE, Department of Physics and Astronomy, McMaster University, T. ITO, P. L. RUSSO, A. T. SAVICI, Y. J. UEMURA, Department of Physics, Columbia University, H. KIM, S. WAKIMOTO, R. J. BIRGENEAU, Department of Physics, University of Toronto — Recent work at Brookhaven was supported by the Office of Science, U.S. Department.

8:48AM A34.00005 The emergence of coherent magnetic excitations in the pseudogap state of underdoped superconducting La_{2-x}Sr_xCuO_4, S. M. HAYDEN, O. J. LIPSCOMBE, B. VIGNOLLE, University of Bristol, T. G. PERRING, C. D. FROST, Rutherford Appleton Laboratory — We use inelastic neutron scattering to measure the magnetic excitations in the underdoped superconductor La_{2-x}Sr_xCuO_4 (x=0.085, T_c=22 K) over wider energy (5 < E < 200 meV) and temperature (5 < T < 300 K) ranges than previously studied.

At low temperatures, the magnetic response is highly structured in energy and momentum with peaks in the local susceptibility /chi/ (E) at 15 and 50 meV and a strongly anisotropic four-peaked structure in /chi/ (q) for E ≈ 185 meV. Raising from T = 30 K to 300 K causes dramatic changes in the response with the observed structure in /chi/ (q, E) for E < 70 meV disappearing and being replaced with a strongly damped response with a characteristic energy scale I' ≈ 50 meV. The results are discussed with respect to the pseudogap present for this composition.

9:00AM A34.00006 Spin Excitations in La_{1.75}Sr_{0.25}Zn_{0.1}Cu_{0.99}O_4, S. M. HAYDEN, O. J. LIPSCOMBE, B. VIGNOLLE, University of Bristol, T. G. PERRING, C. D. FROST, Rutherford Appleton Laboratory — We use inelastic neutron scattering to measure the magnetic excitations in the underdoped superconductor La_{2-x}Sr_xCuO_4 (x=0.085, T_c=22 K) over wider energy (5 < E < 200 meV) and temperature (5 < T < 300 K) ranges than previously studied.

At low temperatures, the magnetic response is highly structured in energy and momentum with peaks in the local susceptibility /chi/ (E) at 15 and 50 meV and a strongly anisotropic four-peaked structure in /chi/ (q) for E ≈ 185 meV. Raising from T = 30 K to 300 K causes dramatic changes in the response with the observed structure in /chi/ (q, E) for E < 70 meV disappearing and being replaced with a strongly damped response with a characteristic energy scale I' ≈ 50 meV. The results are discussed with respect to the pseudogap present for this composition.

9:12AM A34.00007 Magnetic signatures of the pseudogap phase and doping dependence of the antiferromagnetic resonance in HgBa_2Cu_2O_{4+δ}, YUAN LI, Stanford Univ., VICTOR BALEDENT, LLB, France, NEVEN BARI, Univ. Stuttgart, Germany, PHILIPPE BOURGES, LLB, France, YONGCHAN CHO, Pusan National Univ., Korea, BENOIT FAUQUE, ESPCI, France, KLAUDIA HRADIL, Univ. Gottingen, Germany, RICHARD MOLE, Forschungseinrichtung HML, Germany, YVAN SIDIS, LLB, France, GUICHUAN YU, Stanford Univ., XUDONG ZHAO, Jilin Univ., China, MARTIN GREVEN, Stanford Univ. — We present our latest experimental results for the pseudogap phase of the model high-Tc superconductor HgBa_2Cu_2O_{4+δ}. Refinement of our polarized neutron diffraction experiments [Y. Li et al., Nature 455, 372 (2008)] using sizable single-crystals of this structurally simple compound consistently show a novel magnetic order below the pseudogap temperature. Furthermore, DC magnetic susceptibility measurements on the highest-quality crystals exhibit a response with highly anisotropic temperature- and doping-dependence, in which the pseudogap anomaly is only visible when the magnetic field is applied along the c-axis. These findings strongly suggest that the new magnetic order competes with the superconductivity. Building on our initial work for optimally-doped HgBa_2Cu_2O_{4+δ} [G. Yu et al., arXiv: 0810.5759], we also briefly discuss preliminary results for the doping dependence of the antiferromagnetic resonance.
9:24AM A34.00008 Spin correlations and magnetic excitation spectrum of electron-doped Nd$_2$−$\alpha$Ce$_\alpha$Cu$_{2+x}$O$_{4+\delta}$ near the magnetic quantum critical point, EUGENE MOYOYAMA, GUICHUAN YU, YUAN LI, Stanford Univ., DANIEL PETITGRAND, LBL, France, KLAUDIA HRADIL, Univ. Gottingen, Germany, RICHARD MOLE. Forschungszentrum Juelich, Germany, PATRICK MANG, INNA VISHIK, Stanford Univ., OWEN VAJK, Univ. of Missouri-Columbia, MARTIN GREVEN, Stanford University — One of the most intriguing issues in the field of high-T$_c$ superconductivity is the electron-hole asymmetry: the hole- or electron-doping of the parent Mott insulators leads to superconductors with differing properties. For the comparatively less-studied electron-doped materials, the antiferromagnetic phase extends more, leading to a greater magnetic susceptibility and a more prominent effect on the magnetic excitation spectrum. The critical temperature $T_0$ defines the boundary between the magnetic and superconducting phases and is a function of the magnetic doping ratio $x$. The magnetic excitation spectrum shows a peak at $T_0$ and a shoulder at $T_0/\alpha$. The critical current density is calculated for the prepared samples from magnetic hysteresis measurements.

9:36AM A34.00009 Studies of broken time reversal symmetry states in high temperature superconductors using high resolution Sagnac interferometry, ELIZABETH SCHEMM, HOVNATAN KARAPETYAN, Stanford University, JING XIA, California Institute of Technology, MARTIN M. FEJER, AHARON KAPITULNIK, Stanford University — Using a cryogenic fiber Sagnac interferometer, we measure polar Kerr effect to high precision in several high-$T_c$ superconductors, concentrating on YBa$_2$Cu$_{3-x}$O$_{7-y}$. Previous work on YBa$_2$Cu$_{3-x}$O$_{7-y}$ showed non-zero Kerr rotations on the order of $\sim 1$ rad, appearing near the pseudogap temperature $T^*$ and marking what appears to be a true phase transition. We continue this study on single crystals and oriented film to further understand the dependence of the observed Kerr signal on crystal direction, as well as to further probe the anomalous response of this effect to magnetic field training.

9:48AM A34.00010 Giant impact of magnetic impurity on stability of stripe order in high-Tc cuprate, MASAKI FUJITA, Institute for Materials Research, Tohoku University, MASANORI ENOKI, Department of Physics, Tohoku University, SATOSHI IUKUBO, KAZUYOSHI YAMADA, World-Preeminent-International Research Center Initiative, Tohoku University — To study the stability of stripe order in cuprate oxides thought impurity-effect, we performed neutron-scattering experiments on La$_{1.88-x}$Sr$_{0.12+y}$Cu$_{1-x}$M$_x$O$_{4+y}$ ($y=0$ for M=Cu, Zn and $y=0.01$ for M=Ga, Fe). Well-defined incommensurate peaks from charge-density-wave order were observed in the low-temperature-orthorhombic phase (LTO) by impurity substitution, and the scattering intensity is much stronger in the Fe-doped system than in the Zn-doped one. Integrated intensity of magnetic peak from spin-density-wave order was also enhanced by Fe-doping, while it does not change so much by Zn - and Ga- substitutions. These results indicate that the static spin and charge stripe orders can be realized in the LTO phase, and the stability is effectively induced by doping the magnetic impurity.

10:00AM A34.00011 Anomalous normal state magneto-resistance in the noncentrosymmetric superconductor Li$_2$Pt$_x$B$_{1-x}$, B. J. TAYLOR, C. MCELROY, T. A. SAYLES, UCSD, A. C. MOTA, ETH-Zurich, M. BRIAN MAPLE, UCSD — The isotropic superconducting compounds Li$_2$PdB and Li$_2$PtB crystallize in a structure lacking physical inversion symmetry. In contrast to the isotropic symmetry breaking superconductors CePt$_3$Si, CeRhSi$_2$, and UIr, to date, no evidence of magnetic order has been reported in either Li$_2$PdB or Li$_2$PtB. Through detailed magnetoresistive and magnetization measurements of Li$_2$PtB, we have observed behavior suggestive of a link between normal state electronic transport and magnetic properties, and behavior that is indicative of superconducting ground state. Corresponding changes in magnetoresistive and magnetic behavior are found where both properties exhibit two distinct features at high and intermediate temperatures. Remarkably, both features evolve as a function of magnetic field and temperature towards the $T=0$ value of the superconducting upper critical field $H_{c2}(0) \approx 1.5$ T. Polycrystalline samples of Li$_2$PtB, with the highest reported values to date for the superconducting critical temperature, $T_c = 3K$, and residual resistivity ratio, $\rho_{RT} / \rho(0) \approx 2$, were used in this study.

1 Supported by NSF No. DMR-0403491, NHMFL via NSF No. DMR-0654118, US DOE project MA-509-MACA, EURYI Scheme, MEXT-CT-2006-039047 and the National Research Foundation of Singapore.

10:12AM A34.00012 Glassy effects in magnetotransport in La$_{1.97}$Sr$_{0.03}$CuO$_4$ thin films, X. SHI, J. JAROSZYNSKI, D. POPOVICI, Dept. of Phys. & Natl. High Magnetic Field Lab, Florida State Univ., C. PANAGOPoulos, Dept. of Phys., Univ. of Crete and FORTH & Div. of Phys. & Appl. Phys., Nanyang Tech. Univ., G. LOGVENOV, A. BOLLINGER, I. BOZOVIC, Brookhaven Natl. Lab. — We have studied the in-plane magnetoresistance (MR) in atomically smooth, MBE grown La$_{1.97}$Sr$_{0.03}$CuO$_4$ thin films. The MR was measured at temperatures between 0.6 K and 8 K and in $\beta$ up to 9 T, both parallel and perpendicular to the c-axis. The MR exhibits strong dependence on magnetic field history, such as hysteresis and memory at low $T$, similar to the results on c-axis transport in single crystal samples [1]. Here, however, the difference between field-cooled and zero-field cooled MR vanishes above $T=5$ K, independent of the magnitude and orientation of $B$. Low $T$ noise resistance measurements also will be discussed. The results suggest that the glassiness observed in the films may also originate from the slow charge dynamics at low temperatures. [1] I. Raicic et. al., PRL 101, 177004 (2008).

1 Supported by NSF No. DMR-0403491, NHMFL via NSF No. DMR-0654118, US DOE project MA-509-MACA, EURYI Scheme, MEXT-CT-2006-039047 and the National Research Foundation of Singapore.

10:24AM A34.00013 Novel positive magnetoresistance in lightly doped La$_2$CuO$_4$, I. RAICIC, D. POPOVICI, Dept. of Phys. & Natl. High Magnetic Field Lab, Florida State Univ., C. PANAGOPoulos, Dept. of Phys., Univ. of Crete and FORTH & Div. of Phys. & Applied Phys., Nanyang Technological Univ., T. SASAGAWA, Materials and Structures Lab., Tokyo Inst. of Technology — We have measured magnetoresistance (MR) in single crystals of La$_{1.97}$Sr$_{0.03}$CuO$_4$ and La$_2$CuO$_{4+y}$ at temperatures $0.050 \leq \langle T \rangle \leq 70$ K and fields $B(\leq 1.5 T)$ parallel and perpendicular to the c-axis. Our previous inelastic neutron scattering measurements show that in the compound Nd$_{2-}Ce_{\alpha}$Cu$_{2+x}$O$_{4+\delta}$, genuine long-range antiferromagnetism does not extend as far as traditionally thought, and may not coexist with bulk superconductivity; the system features a magnetic quantum critical point at $x \approx 0.13$, very close to the composition above which superconductivity is first observed [Motyama et al., Nature 445, 186 (2007)]. Here we present new measurements for the instantaneous spin correlations and the magnetic excitation spectrum that aim to refine our understanding of the physics in this interesting doping regime.

1 Supported by NSF No. DMR-0403491, NHMFL via NSF No. DMR-0654118, US DOE project MA-509-MACA, EURYI Scheme, MEXT-CT-2006-039047 and the National Research Foundation of Singapore.

10:36AM A34.00014 Magnetic hysteresis studies of Ti-2223 substituted by Fe and Zn , AY ABOU-ALY, RAMADAN AWAD, IBRAHIM IBRAHIM, Faculty of Science, Alexandria, Egypt, AHMED FARAJ, Physics Department, Faculty of Science, BAU University, Beirut, Lebanon — Effect of Fe and Zn substitutions on the magnetic hysteresis of Ti-2223 are investigated in high magnetic fields up to 9 Tesla and at different temperatures $(T= 5$, 60 and 80 K). The results of magnetic hysteresis loops show that the area of these loops decreases as Fe-content increases, whereas it increases for Zn-substitutions till $x = 0.2$ and then decreases for $x > 0.2$. The magnetization difference $\Delta M$ is found to decay exponentially with temperature at low magnetic fields, according to $\Delta M \propto \exp (-T/T_0)$. The characteristic temperature $T_0$ is found to be varied from 6 K to 40 K and it is related to the applied magnetic field $B$ according to $T_0 \propto B^{-1/n}$. The critical current density is calculated for the prepared samples from magnetic hysteresis measurements and compared with that determined from ac magnetic susceptibility. The results are discussed according to the flux motion and flux pinning.
10:48AM A34.00015 Neutron Scattering Study of Magnetic Field Effect on the Stripe Order in LBCO. ZHI JUN XU, JINSHEWEN WEN, GUANGYONG XU, MARKUS HÜCKER, JOHN TRANQUADA, GENDA GU, BNL. BNL NEUTRON SCATTERING GROUP TEAM — We have been investigating the relationship of stripe order to high-temperature superconductivity in cuprates. In particular, our neutron scattering results indicate that spin-stripe order is present in La$_2$-Ba$_x$CuO$_4$ (LBCO) over a substantial range of doping about x = 1/8, where the bulk superconductivity is anomalously suppressed. Focusing on the x = 1/8 composition, we have recently studied the impact on stripe order of a magnetic field applied along the c-axis [1]. Applying a field up to 7 T, we observed a small enhancement of the intensity of the incommensurate antiferromagnetic superlattice peaks and a slight increase in the ordering temperature. In measurements of the spin dynamics, the field had no significant impact on the small spin gap (∼ 0.5 meV) found in the ordered phase [2]. [1] Jinshew Wen et al., arXiv:0810.4085. [2] J.M. Tranquada et al., arXiv:0809.0711. Work supported by Office of Science, U.S. DOE, under Contract No. DEAC02-98CH10886.

Monday, March 16, 2009 8:00AM - 11:00AM —
Session A35 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors I: Synthesis and New Materials 405

8:00AM A35.00001 Superconductivity in layered pnictides BaIr$_2$P$_2$ and BaRh$_2$P$_2$. DAIGOROU HIRAI, TOMOHIRO TAKAYAMA, Dept. of Advanced Materials, Univ. of Tokyo, RYUJI HIGASHINAKA, HIROKO ARUGA-KATORI, Riken, HIDENORI TAKAGI, Dept. of Advanced Materials, Univ. of Tokyo — The exploration of new superconductors, triggered by the discovery of LaFeAsO(O,F), has concentrated mostly on Fe-based pnictides. A variety of non-Fe pnictides, isostructural to Fe pnictide superconductors, have been known for a long time but not yet fully explored in terms of possible superconductivity. Further exploration of non-Fe pnitride superconductors is important for understanding the key factors in realizing the high Tc in the Fe pnictides. We report new Ir and Rh pnictide superconductors, isostructural to BaFe$_2$As$_2$, BaRh$_2$P$_2$ and BaIr$_2$P$_2$, with Tc = 1.0 and 2.1 K respectively. This discovery demonstrates the presence of superconductivity over a surprisingly broad range of transition metal compounds with ThCr$_2$Si$_2$-type structure from Fe to Ir.

8:12AM A35.00002 Superconductivity and enhanced susceptibility in SrFe$_2$As$_2$ single crystals. S. R. SAHA, N. P. BUTCH, K. KIRSHENBAUM, J. PAGLIONE. Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — Single crystals of SrFe$_2$As$_2$ grown using a self-flux solution method were characterized via x-ray, transport, magnetization and specific heat studies, revealing a superconducting transition at 21 K which appears far below the magnetostructural transition at 198 K as evidenced by transitions in resistivity and susceptibility. We present experiments which probe the nature of this phase and its relation to the enhancement of magnetic susceptibility in superconducting samples.


3Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

8:36AM A35.00004 Transport, magnetic and thermal properties of MFePO M = La, Pr, and Nd single crystals. RYAN BAUMBACH, JAMES HAMLIN, LEI SHU, DIEGO ZOCCO, NICOLE CRISOSTO, M. BRIAN MAPLE, Department of Physics and IPAPS, University of California, San Diego — The recent discovery of Tc values near 26 K in the compound LaFeAsO$_1-x_F$ induced a torrent of publications on what are now recognized as a new class of Fe-based high temperature superconductors. To date, the phosphorus based versions of these compounds have received little attention due to their comparatively low Tc values. In this work we report the low temperature electrical resistivity, magnetic susceptibility, and specific heat data of single crystalline PrFePO and NdFePO. We also report the effect of annealing on the properties of LaFePO, PrFePO, and NdFePO. A systematic comparison of the occurrence of superconductivity in the series MFePO and MFeAsO (where M is a lanthanide) points to a possible difference in the origin of the superconductivity in these two series of compounds.

3This research was supported by the U.S. Department of Energy (DOE) under Research Grant # DE-FG02-04ER46105 and Research Grant # DE-FG02-04ER46178 and by the National Science Foundation (NSF) under Grant # DMR0802478.

4Student was a participant in the Research Experience for Undergraduates (REU) program at UCSD

8:48AM A35.00005 New ternary phosphide superconductors with the ThCr2Si2 parent structure. NICHOLAS BERRY, CIGDEM CAPAN, University of California Irvine, GABRIEL SEYFARTH, Université de Montréal, University of California Irvine, ZACHARY PISK, University of California Irvine — Compounds with the ThCr2Si2 structure have been studied extensively for over 20 years for their interesting magnetic, superconducting, and heavy fermion properties. We have grown single crystals of new ternary phosphides in this structure in the form of AX2P2, with A being an Alkaline Earth Metal and X a transition metal. We have characterized the properties of these new materials with X-ray, heat capacity, resistivity, and susceptibility measurements and have discovered new superconductors.

9:00AM A35.00006 Magnetic, Thermodynamic, and Transport Properties of Layered Arsenides BaRu$_2$As$_2$ and SrRu$_2$As$_2$. R. NATH, Y. SINGH, D.C. JOHNSTON, Ames Lab. and Dept. of Phys. and Astronomy, Iowa State University, Ames, IA 50011, USA — As part of our effort to search for novel superconductors related to the FeAs high-Tc superconductors, we have synthesized polycrystalline samples of BaRu$_2$As$_2$ and SrRu$_2$As$_2$. The magnetic, transport and thermodynamic properties of the samples were investigated by means of magnetic susceptibility χ(T), electrical resistivity ρ(T), and heat capacity C(T) measurements. The temperature dependence of ρ indicates metallic character for both compounds with a residual resistivity ratio ρ(310 K)/ρ(2 K) of 17 and 7 for the Ba and Sr compounds, respectively. The Cp(T) results indicate a low density of states at the Fermi level with the low-T Sommerfeld coefficient γ ≈ 4.9 and 4.13 mJ/mole K$^2$ for the Ba and Sr compounds, respectively. The Debye temperature θD was estimated to be 270 K and 260 K for the Ba and Sr compounds, respectively. The χ(T) was found to be diamagnetic with a small absolute value for both the compounds. No evidence for superconductivity, a spin density wave, or a structural transition was observed from the C(T) and ρ(T) measurements down to 2 K. However, the χ(T) data for SrRu$_2$As$_2$ exhibit a cusp at ∼ 190 K, possibly an indication of a structural and/or magnetic transition.
9:12AM A35.00007 Robust Ferromagnetism in Ultrathin Films of CeFeAsO

9:24AM A35.00008 Reaction Kinetics of the Formation of SmFeAsO$_{1-x}$F$_x$ High $T_c$ Superconductor Probed by High Energy X-ray Diffraction

9:36AM A35.00009 Growth and Properties of SmFeAsO$_{1-x}$Fx thin films using pulsed laser deposition

9:48AM A35.00010 Superconducting Fe-Based Compounds (A$_{1-x}$Sr$_x$)$_2$Fe$_2$As$_2$ with A = K and Cs with Transition Temperatures up to 37 K.

10:00AM A35.00011 The superconductivity in alkaline containing iron arsenide system.

10:12AM A35.00012 Superconductivity in Sr-122 Iron Arsenide System by Yttrium Doping.

10:24AM A35.00013 High-pressure growth of SmFeAsO$_{1-x}$ single crystals without fluorine doping.
10:36AM A35.00014 Growth of superconducting FeSe films, MICHI NAITO, SHINYA AGATSUMA, SHINYA UEDA, Tokyo University of Agriculture and Technology, TAT TEAM — The recently discovered Fe arsenide and chalcogenide superconductors have provided the superconducting community with a great surprise that Fe-based compounds are not ferromagnetic but superconducting with high Tc. The superconducting Fe arsenides and chalcogenides are also interesting from the viewpoint of superconducting electronics. One can see good lattice compatibility between the superconducting Fe family and the existing III-V and II-VI semiconducting family (GaAs, ZnSe). All-epitaxial super-semiconductor multilayer structures may be ideal for superconducting heterostructures. For this reason we have attempted to grow epitaxial thin films of the superconducting Fe family. Of this family, tetragonal α-FeSe seems to be the easiest to grow thin films. We employed two approaches for FeSe film growth: post-annealing and MBE growth. In the post-annealing, precursor films of Fe are annealed at 500 - 600 °C with Se vapor in an evacuated quartz tube. Annealing with elemental Se produced superconducting FeSe. In the in situ growth, precursor films of Fe were annealed at 500 - 600 °C with Se vapor in an evacuated quartz tube. Annealing with elemental Se produced superconducting FeSe, whereas annealing with Se polycrystalline pellets produced superconducting FeSe with Tc(onset) ~ 10 K. In the MBE growth, we attempted the growth similar to GaAs growth, namely with the vapor rich in Se, expecting self-limiting adsorption of Se. MBE films so far obtained with the growth temperature of 330 °C are nonsuperconducting hexagonal β-FeSe.

10:48AM A35.00015 In situ X-ray Synchrotron Diffraction Study of the Synthesis of LaFeAsO and LaFeAsO1−xFx, R.W. MCCALLUM, Ames Laboratory, Materials Science and Engineering, Iowa State University, Ames, IA 50011, J.-Q. YAN, G.E. RUSTAN, E.D. MUN, S. DAS, R.C. NATH, YOUWEN XU, S.L. BUD’KO, K.W. DENNIS, Ames Laboratory, US DOE, Ames Laboratory, Iowa State University, Ames, IA 50011 — The reaction path for the synthesis of LaFeAsO and LaFeAsO1−xFx by nominally solid state reaction was studied in situ x-ray synchrotron diffraction technique and Differential Thermal Analysis (DTA) in the temperature interval 100 °C ≤ T ≤ 1150 °C. Starting materials were La2As2, Fe3O4, Fe and for the F containing materials LaF3. The results show that the synthesis is characterized by three temperature intervals: (1) below 400 °C, Fe3O4 gradually transforms to FeO. (2) In the temperature interval 400 °C < T < 800 °C, multiple intermediate reactions take place resulting in the formation of La2O3 and FeAs compounds. (3) above 800 °C, reaction leads to the formation of LaFeAsO. Possible reaction paths and the difference between F-free and F-doped samples will be discussed in the talk.
Signals of a Carbon Nanotube Field-Effect Transistor, and discuss the contact effect of the electrodes on the transport properties. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties. To detect electric signals through nanotubes, electrodes must be connected to the nanotubes. The contact with the electrodes sensitively influences their electronic structures and transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculations that include the effect of the contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties.

 Signals of a Carbon Nanotube Field-Effect Transistor, and discuss the contact effect of the electrodes on the transport properties. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties. To detect electric signals through nanotubes, electrodes must be connected to the nanotubes. The contact with the electrodes sensitively influences their electronic structures and transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculations that include the effect of the contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties.

 Electric signals are detected by a gate voltage applied to a gate electrode bridged between metallic electrodes on a carbon nanotube, and discuss the contact effect of the electrodes on the transport properties. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties. To detect electric signals through nanotubes, electrodes must be connected to the nanotubes. The contact with the electrodes sensitively influences their electronic structures and transport properties. Therefore, it is important to discuss the transport properties on the basis of the detailed electronic state calculations that include the effect of the contact with the electrodes. We have investigated quantum transport in carbon nanotubes bridged between metallic electrodes on a gate electrode, and discuss the contact effect of the electrodes on the transport properties.
10:12AM A36.00012 Tuning the electronic states of carbon nanotube based devices under magnetic field. SEBASTIEN NANOT, LNCMP - Laboratoire National Des Champs Magnetiques Pulses, BERTRAND RAQUET, WALTER ESCOFFIER, JEAN-MARC BROTO, LNCMP, REMI AUVILLER, STEPHAN ROCHE, CEA - INAC/SPSMS/GT — Carbon nanotubes have already demonstrated their wide potential in nanoelectronics and optoelectronics. In our study, we demonstrate that an applied magnetic field, along with a control of the electrostatic doping, drastically modifies the electronic band structure of a carbon nanotube based transistor. Several examples will be addressed in this presentation. In a parallel configuration (B parallel to the tube axis), a quantum flux threading the tube induces a giant Aharonov-Bohm conductance modulation mediated by Schottky barriers which profile is magnetic field dependent. In the perpendicular configuration, the applied magnetic field breaks the revolution symmetry along the circumference and non conventional Landau states are expected in the high field regime. By playing with a carbon nanotube based electronic Fabry-Perot resonator, we bring evidence that the electronic transmission of the device can be modified by a transverse magnetic field. The field dependence of the resonant states of the cavity reveals the onset of the first landau state at zero energy. These experiments also enlighten the outstanding efficiency of magneto-conductance experiments to probe the electronic properties of carbon based nano-materials.

10:24AM A36.00013 Transport and Magnetism in Template Synthesized Hydrogenated Multiwalled Carbon Nanotubes. ADAM FRIEDMAN, Northeastern University Department of Physics, HYUNKYUNG CHUN, Northeastern University Department of Mechanical and Industrial Engineering, DONALD HEIMAN, Northeastern University Department of Physics, YUNG JOON JUNG, Northeastern University Department of Mechanical and Industrial Engineering, LATIKA MENON, Northeastern University Department of Physics — In this work, we synthesize highly disordered carbon nanotubes by CVD in porous alumina templates. We show that, due to the disorder in the nanotubes, they can easily be made to uptake hydrogen by annealing. We show that this induces ferromagnetism in the nanotubes, and we perform a magnetic study. We also measure the transport properties of the nanotubes. First, we find a rate dependent hysteretic magnetoresistance. We explain the rate dependence through strong magneto-viscosity effects, and we attribute the hysteresis to anisotropic magnetoresistance. We also discover a magnetic field-driven temperature dependent transition from positive to negative magnetoresistance in the ferromagnetic nanotubes that is not observed in similarly disordered un-hydrogenated carbon nanotubes. We attempt to explain this behavior by considering it an order-disorder transition described by the Bright model due to several scattering pathways, that are present in the ferromagnetic nanotubes that are not present in the non-ferromagnetic tubes.

10:36AM A36.00014 Magnetotransport of hybrid nanoparticle-nanowire systems1, DONGKYUN KO, COLE ROBINETTE, XIANWEI ZHAO, FENGYUAN YANG, EZEKIEL JOHNSTON-HALPERIN, The Ohio State University — Semiconductor nanowires decorated with metal nanoparticles have a number of interesting electronic and photonic properties. For example, top-gated field effect transistors based on these hybrid systems have shown charge storage when operated in a floating-gate architecture. In addition, recent measurements have demonstrated that spin relaxation and phase coherence lengths can be extracted from magnetococonductance patterns in the gating response of bare nanowires. Together, these results suggest the possibility of in situ tuning of the spin relaxation length in hybrid systems via modulation of the floating-gate potential. Initial efforts along these lines will be presented, including gating response and low temperature magnetotransport in 50 nm diameter InP nanowires decorated with Au nanoparticles from 20 – 250 nm in diameter. The potential utility of these systems as testbeds for the exploration of spin scattering and transport will be discussed.

1Partial funding for this research was provided by the Center for Emergent Materials at the Ohio State University, a NSF MRSEC (Award Number DMR-0820414).

10:48AM A36.00015 Exploration of conductance peak splitting in carbon nanotube field effect transistors at critical field strengths. JEFFREY D. STEPHENS, JEROME C. LICINI, Lehigh University, A.T. CHARLIE JOHNSON, DOUG R. STRACHAN, DANVERS E. JOHNSTON, SAM KHAMIS, University of Pennsylvania — Carbon nanotube field effect transistors were produced by chemical vapor deposition growth of nanotubes on oxidized silicon substrate. Samples were back gated on doped silicon and contacted with gold/chrome contacts. Conductance measurements were performed at low temperature and high magnetic field using a dilution refrigerator and a superconducting magnet. Data was taken at 0.5 Tesla increments from 0-11Tesla. The differential conductance (dI/dV) shows an interesting asymmetry with bias voltage as well as a near zero bias conductance peak. The near zero bias conductance peak demonstrates splitting at two critical magnetic field strengths on the 0.5T scale. These two critical regimes are further explored on a finer magnetic field scale.

Monday, March 16, 2009 8:00AM - 11:00AM — Session A37 DCP: Focus Session: Fundamental Developments in Density Functional Theory I

8:00AM A37.00001 Insights and Progress in Density Functional Theory. WEITAO YANG1, Duke University — Density functional theory of electronic structure is widely and successfully applied in simulations throughout engineering and sciences. However, there are spectacular failures for many predicted properties, which can be traced to the delocalization error and static correlation error of commonly used approximations. These errors include understimation of the barriers of chemical reactions, the band gaps of materials, the energies of dissociating molecular ions and charge transfer excitation energies. Typical DFT calculations also fail to describe degenerate or near degenerate systems, as arise in the breaking of chemical bonds, and strongly correlated materials. These can all be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. Understanding the errors of functionals in the simplest way possible — as violations of exact conditions for fractional charges and fractional spins — opens the path forward for reduction of the errors and for applications of density functional theory in new frontiers. [P. Mori-Sanchez, A. J. Cohen, and W. T. Yang, Phys. Rev. Lett. 100:146401(2008); Phys. Rev. B,77:115123(2008); J. Chem. Phys. 129:121104(2008); Science, 321:792(2008)]

1in collaboration with A. J. Cohen, P. Mori-Sanchez, and E. R. Johnson

8:36AM A37.00002 Semiclassical origins of density functional theory1. KIERON BURKE, University of California, Irvine — Until the seminal work of Hohenberg, Kohn, and Sham of the mid 60’s, most density functional theory (DFT) was derived from semiclassical approximations. This non-empirical approach shows an intrinsic difference between solids (for which DFT was originally developed) and molecules, and explains many of its more mysterious manifestations. For example, the success of DFT for molecules has nothing to do with the uniform gas. Results include [1] a derivation of the empirical parameter in the B88 exchange functional, [2] PBesol, a new GGA that restores the exchange gradient expansion and improves the band gaps of materials, the energies of dissociating molecular ions and charge transfer excitation energies. Typical DFT calculations also fail to describe degenerate or near degenerate systems, as arise in the breaking of chemical bonds, and strongly correlated materials. These can all be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. Understanding the errors of functionals in the simplest way possible — as violations of exact conditions for fractional charges and fractional spins — opens the path forward for reduction of the errors and for applications of density functional theory in new frontiers. [P. Mori-Sanchez, A. J. Cohen, and W. T. Yang, Phys. Rev. Lett. 100:146401(2008); Phys. Rev. B,77:115123(2008); J. Chem. Phys. 129:121104(2008); Science, 321:792(2008)]]

1Research Supported by NSF grant CHE-0809859.
In order to study spin-orbit coupled systems, spin-transfer torque devices, or even systems with pseudospin coupling like graphene, non-Abelian vector potentials: the Local Approximation.


1. This work supported by NSF Grant No. DMR-0705460.

1. Supported by Robert A. Welch Foundation.

1. NSF CHE-0809859

1. NSF CHE-0809859

1. NSF CHE-0809859

1. National Science Foundation, CHE-0809859
10:48AM A37.00011 Density Functional with Full Exact Exchange, Balanced Nonlocality of Correlation, and Constraint Satisfaction\footnote{Supported by NSF.}. JOHN P. PERDEW, Physics, Tulane U., VIKTOR N. STAROVEROV, Chemistry, U. of Western Ontario, JIANMIN TAO, Los Alamos National Lab, GUSTAVO E. SCUSERIA, Chemistry, Rice U. — We construct a nonlocal density functional with full exact exchange, while preserving the constraint-satisfaction approach and justified error cancellations of simpler semilocal functionals. This is achieved by interpolating between different approximations suitable for two extreme regions of the electron density. In a “normal region”, the exact exchange-correlation hole around an electron is semilocal because its range is reduced by correlation and because it integrates over a narrow range to −1. “Abnormal” regions, where nonlocality is included, allow those in which exchange can dominate correlation (one-electron, nonuniform high density, and rapidly-varying limits), and those open systems of fluctuating electron number over which the exact exchange-correlation hole integrates to a value greater than −1. Regions between these extremes are described by a local hybrid exact semilocal exchange locally.

Monday, March 16, 2009 8:00AM - 11:00AM
Session A38 DCP: Focus Session: The Chemical Physics of Biological and Biologically-inspired Solar Energy Harvesting

8:00AM A38.00001 Investigation of Excitonic Coherence in LHCII by 2D Electronic Spectroscopy\footnote{Supported by the Department of Energy and the National Science Foundation}. TESSA CALHOUN, University of California, Berkeley — Photosynthesis has evolved with the ability to transfer energy through a matrix of light-harvesting pigment-protein complexes with almost no loss. The accomplishment of this near unity quantum efficiency is a feat that man has yet to understand or replicate. One proposed mechanism integral to this process requires long-lived coherent superpositions of the excitons, delocalized electronic excitations, in these systems. Two-dimensional Fourier transform electronic spectroscopy, already proven to be an ideal technique for investigating these coherences, has been employed to study Light Harvesting Complex II (LHCII), the most abundant light harvesting complex in higher plants. As in other photosynthetic systems previously studied, we observe long-lived coherence lasting beyond many of the excitons’ lifetimes. Furthermore, unique coherence signatures allow the energies of the individual excitons to be located in an otherwise highly congested spectrum. This technique, by which 2D FT electronic spectroscopy can pinpoint excitonic spectral positions, and the resulting implications for LHCII will be discussed.

8:36AM A38.00002 Luminous Solar Concentrators Employing Phycobilisomes\footnote{In collaboration with: Shaul Mukamel, University of California, Irvine}. MARC BALDO, MIT — At current manufacturing growth rates, it is expected to take at least 20 years to produce enough Si-based solar cells to make a significant impact on the world energy supply. Solar concentrators can alleviate manufacturing constraints by focusing light on small solar cells. Luminous solar concentrators (LSCs) are especially promising because they do not need to track the sun to obtain high optical concentration factors. Light incident on an LSC is absorbed by dyes, re-emitted into a guided mode in the slab, and finally collected by a PV cell mounted at the edge of the slab. The maximum optical concentration of an LSC is theoretically limited by the wavelength shift between absorption and emission in the dye. In this presentation, we describe LSCs that mimic a four energy level laser design, maximizing the wavelength shift and minimizing re-absorption losses. We employ phycobilisomes - photosynthetic antenna complexes that concentrate excited states in red algae and cyanobacteria. The phycobilisomes are cast in a solid-state matrix that preserves their internal Frster energy-transfer pathways and large wavelength shift between absorption and emission. Casting is a simple fabrication technique that also eliminates any need for expensive high-index glass or plastic. By comparing the performance of intact and decoupled complexes, we establish that energy transfer within intact phycobilisomes reduces LSC self-absorption losses by approximately (48±5)%. These results suggest that phycobilisomes are the model for a new generation of cast LSCs with improved efficiency at high optical concentrations.

9:12AM A38.00003 Coherent Multidimensional Spectroscopy of Photosynthetic Complexes: Manipulating Quantum Pathways by Optical Pulse Sequences\footnote{In collaboration with: Darius Abramavicius and Dmitri Voronine, University of California, Irvine}. DARIUS ABRAMAVICIUS\footnote{1}, University of California, Irvine — The response of chromophores aggregates to sequences of femtosecond laser pulses is simulated using the nonlinear excitation equations. The nonlinear response can be interpreted in terms of the scattering of elementary excitations, quasiparticles, rather than as transitions among eigenstates. Applications are made to the Fenna-Matthews-Olson (FMO) and the PSI light harvesting complexes. Some fundamental symmetries of multidimensional optical signals are used to design techniques that can selectively resolve coherent quantum dynamics and incoherent energy dissipation. Simulations show damped oscillations of cross peaks corresponding to evolution of coherences, without interference from incoherent population relaxation. Energy transfer pathways are seen through the redistribution of crosspeak amplitudes. Resolution is enhanced by employing specific pulse polarization configurations to generate chirality-induced signals. New pulse sequences are designed to generate signals that are induced by correlations among elementary excitations. Specific phase-matching directions can target the correlated dynamics of double excitations. Cross peaks in 2D correlation plots are interpreted in terms of quasiparticle scattering and shown to reveal the double-exciton wavefunction, projected into products of single-excitations. Uncorrelated double-exciton states do not show up in the spectra due to quantum interference among pathways. The proposed techniques amplify cooperative dynamical features and reveal information on the robustness of quantum states to fluctuating environments. In collaboration with Darius Abramavicius and Dmitri Voronine, University of California, Irvine, CA 92697.

9:48AM A38.00004 Exploring Nanophotovoltaic Molecules using STM\footnote{In collaboration with: Shaul Mukamel, University of California, Irvine}. CHENGGANG TAO, University of California at Berkeley, JIBIN SUN, XIAOWEI ZHANG, R. YAMACHIKA, D. WEGNER, Y. BAHRI, G. SAMSONIDZE, S. LOUIE, T. TILLY, R. SEGALMAN, M. CROMMIE — Composite molecular solar cells are a promising and exciting alternative to traditional silicon or gallium arsenide solar cells, but the power conversion efficiency remains low. In order to further increase this efficiency, a deeper understanding of the microscopic mechanisms at work in organic solar cells is needed. Using scanning tunneling microscopy and spectroscopy we have investigated nanophotovoltaic molecules that combine both donor and acceptor elements. Submolecular spectral resolution reveals the energy level alignment within these composite molecular structures. This information should be useful for understanding the energy conversion pathways within molecular solar cells, and for developing higher efficiency solar cell materials.

10:00AM A38.00005 New highly polar semiconductor ferroelectrics for solar energy conversion devices\footnote{Supported by the Department of Energy and the National Science Foundation}. ANDREW M. RAPPE, ILYA GRINBERG, JOSEPH W. BENNETT, University of Pennsylvania — Solar energy is a promising long-term solution for future energy requirements; however, current solar energy conversion devices are plagued by low efficiency. The use of ferroelectric ABO$_3$ perovskite oxides is one approach for boosting conversion efficiency. Ferroelectric oxides possess spontaneous polarization and have been shown to produce a bulk photovoltaic effect, in which charged carriers, specifically electrons and holes, separate to prevent recombination. Once separated, the high-energy electrons are available for electrical work or for the catalytic splitting of water into hydrogen and oxygen. Currently, most solid oxide ferroelectrics have a band gap of at least 3 eV, absorbing primarily in the ultra-violet (UV) region. Since UV light comprises only 8% of the solar spectrum, new materials with a decreased band gap and large polarization would be highly desirable. We use first-principles density functional theory (DFT) calculations to investigate the ground state structures of PbTiO$_3$ solid solutions containing Ni, Pd and Pt. We predict that these proposed materials will display a decreased band gap when compared to PbTiO$_3$, while maintaining or enhancing polarization. They are promising candidates for use as semi-conducting ferroelectric substrates for solar conversion devices.
Non-Markovian process. This efficiency measure has applications to the study of the quantum transport efficiency and engineering of light-harvesting devices.

We derive a new method for computing the Förster coupling between nanoparticles in an arbitrary electrostatic environment. We calculate the self-consistent electronic structure of an exciton, including the electron-hole attraction, in a nanoparticle within the two band effective mass approximation. Self-interaction of the electron and the hole are removed and the eigenstate is approximated as a product state of the electron and hole wavefunctions. The environment is incorporated via boundary conditions on Poisson’s equation and arbitrary dielectric background. The transfer rate of the exciton via Förster coupling to a neighboring nanoparticle is computed, without making a dipole approximation, from the results of the self-consistent calculation. Departure from the usual $1/R^3$ dependence are calculated, as well as specific cases where gates or additional nanoparticles are present.

Non-Markovian Environmental Contributions to the Efficiency of Energy Transfer. CESAR RODRIGUEZ-ROSARIO, PATRICK REBENTROST, ALAN ASPURU-GUZIK. Harvard University — Non-Markovian environmental contributions of the environment to the efficiency of energy transfer by considering a non-Markovian environment and its interplay with the system Hamiltonian. We focus on the role of memory effects of different orders in time, and their competition that affect the energy transfer by defining the efficiency of the non-Markovian process. This efficiency measure has applications to the study of the quantum transport efficiency and engineering of light-harvesting devices.

Spatially correlated fluctuations and coherence dynamics in photosynthesis. Z. G. YU, M. A. BERDING, SRI International, HAOBIN WANG, New Mexico State University — Recent multicolor photon-echo experiments revealed a long-lasting quantum coherence between excitations on donor and acceptor in photosynthetic systems. Identifying the origin of the quantum coherence is essential to fully understand photosynthesis. Here we present a generic model in which a strong intermolecular steric restoring force in densely packed pigment-protein complexes results in a spatial correlation in conformational (static) variations of chromophores, which in turn induces an effective coupling between high-frequency (dynamic) fluctuations in donor and acceptor. The spatially correlated static and dynamic fluctuations provide a favorable environment to maintain quantum coherence, which can consistently explain the photon-echo measurements [1].

This work was supported by the U.S. Army Research Office under Contract W911NF05C0070. HW also acknowledges the support from the National Science Foundation CAREER award CHE-0348956.

**Monday, March 16, 2009 8:00AM - 11:00AM**

**Session A39 DBP: Cellular Biomechanics**

**8:00AM A39.00001** Loss of an actin crosslinker uncouples cell spreading from cell stiffening on gels with a gradient of stiffness. QI WEN, Department of Physics, University of Pennsylvania, FITZROY J. BYFIELD, Institute for Medicine and Engineering, University of Pennsylvania, KERSTIN NORDSTROM, Department of Physics, University of Pennsylvania, PAULO E. ARRATIA, Departments of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, R.TYLER MILLER, Departments of Medicine and Physiology, Case-Western Reserve University, PAUL A. JANMEY, Institute for Medicine and Engineering, Departments of Physics, Engineering, University of Pennsylvania — We use microfluidics techniques to produce gels with a gradient of stiffness to show the essential function of the actin crosslinker filamin A in cell responses to mechanical stimuli. M2 melanoma cells null for filamin A do not alter their adherent area in response to increased substrate stiffness when they link to the substrate only through collagen receptors, but change adherent area normally when bound through fibronectin receptors. In contrast, filamin A-replete A7 cells change adherent area on both substrates and respond more strongly to collagen 1-coated gels than to fibronectin-coated gels. A7 cells alter their stiffness, as measured by atomic force microscopy, to match the elastic modulus of the substrate immediately adjacent to them on the gradient. M2 cells, in contrast, maintain a constant stiffness on all substrates that is as low as that of A7 cells on the softest gels achievable (1000 Pa). By contrasting the responses of these cell types to different adhesive substrates, cell spreading can be dissociated from stiffening.

**8:12AM A39.00002** Substrate Induced Osteoblast-Like Differentiation of Stromal Stem Cells. JACQUELINE BELIZAR, Miller Place High School, REENA GLASER, MATTHEW HUNG, Smithtown High School West, MARCIA SIMON, VLADIMIR JURUKOVSKI, MIRIAM RAFAILOVICH, Stony Brook University, ALICE SHIH — We have demonstrated that Adipose-derived stem cells (ASCs) can be induced to biomineralize on a polybutadiene (PB) coated Si substrate. The cells began to generate calcium phosphate deposits after a five-day incubation period in the absence of dexamethasone. Control cells plated on tissue culture PS culture dish (TCP) did not biomineralize. In addition, the biomineralizing culture retained proliferative cells In order to determine whether the induction was transient, we transferred the cells exposed to polybutadiene after 14 and 28-day incubation periods to TCP dishes. These cells continued to biomineralize. Genetic testing is underway which will determine whether differentiation is maintained after transfer.

**8:24AM A39.00003** Mechanical anisotropy of viscoelasticity in biological cells. MING-TZO WEI, H.D. OU-YANG, Lehigh University — The mechanism that biological cells use to remodel their cytoskeletal structure in response to external stress is unclear. Experimental observations suggest that the cells remodel their skeleton in a manner that is directionally responsive to the external stress. In order to understand these directional responses, we developed a method to measure the rheological response of the cell in orthogonal directions simultaneously. To achieve controlled stimulation and detection, we used a dual-beam optical tweezers, which used a pump and probe scheme to measure the storage and loss modulus of the cellular cytoskeleton. The pump was used to manipulate extracellular micro-particles which were attached to the actin cytoskeleton through trans-membrane integrin alpha receptors. By measuring two independent regions of the cell, we were able to generate a localized mechanical stress on the outer surface of the cell while observing the directionally specifically inside response.
8:36AM A39.0004 Traction forces associated with shape changes in migrating amoeboid cells  
BALDOMERO ALONSO-LATORRE, JUAN C. DEL ALAMO, EBBIE BASTOUNIS, RUDOLPH MEILI, RICHARD FIRTÉL, JUAN C. LASHERS — University of California, San Diego — Amoeboid motility results from the repetition of a repertoire of shape changes (motility cycle). We studied the dominant changes and their relation to the activity and localization of cytoskeletal proteins by applying Principal Component Analysis (PCA) to measurements of cell shape, traction forces and F-actin concentration in migrating Dictyostelium cells. Using wild-type cells (wt) as reference, we investigated myosin II activity by studying myosin II-null (mhc-) and essential light chain-null cells (mhc-). Only three PCA modes are enough to represent 67% of the variance of cell area: dilation/elongation, a half-moon shape and a bulging of the front/back. These modes are similar for wt, mhc- and mhc- but they are implemented more slowly in mhc-. The second mode, which represents sideways protrusion/retraction and is associated to lateral asymmetry in the traction forces, is significantly less important in mhc-.

These results suggest that migration speed decreases in the absence of myosin II due to a reduced control on the spatial organization of the cell stresses.

8:48AM A39.0005 Imaging spatiotemporal redistribution of cellular traction stesses during fibroblast migration on a physiologically relevant ECM mimic  
ZHI PAN, YAJIE LIU, KAUSTABH GHOSH, Stony Brook University, DHRUV NANDAMUDI, Monta Vista High School, DANNY STEPP, North Shore Hebrew Academy High School, TOSHIKO NAKAMURA, RICHARD CLARK, MIRIAM RAFAILOVICH, Stony Brook University — To better understand the dynamics of cell migration, we measured the spatiotemporal redistribution of cellular traction stresses during fibroblast migration at a submicron level and correlated it with nuclear translocation on a physiologically relevant ECM mimic. We found that nuclear translocation occurred in pulses whose magnitude was larger on the low ligand density surfaces (LLDS) than on the high ligand density surfaces (HLDS). Large nuclear translocations only occurred on LLDS when the rear traction forces completely relocated to a posterior nuclear location, while such relocation took much longer time on HLDS, probably due to the greater magnitude of traction forces. Our results suggest that the reinforcement of the traction forces around the nucleus is a critical step during fibroblast migration, serving as a speed regulator, which must be considered in any dynamic molecular reconstruction model of tissue cell migration. A traction gradient foreshortening model was proposed to explain how the relocation of rear traction forces leads to pulsed fibroblast migration.

9:00AM A39.0006 Achieving in-vitro axonal polarization by using micro-patterns  
SOPHIE ROTH, INSTITUT NEEL, MCBT ET CRETA, CNRS GRENOBLE — IN, INSERM UMR 836, JACQUES BROCARD, SYLVIE GORY-FAURE, GIN, INSERM UMR 836, CATHERINE VILLARD, INSTITUT NEEL, MCBT ET CRETA, CNRS GRENOBLE — Our project is based on the elaboration of in vitro neuron networks as simplified models to explore the relation between neuronal architecture and biological function. Beyond a control of soma and neurite position, our first goal was to achieve in-vitro axonal differentiation of embryonic E18 hippocampal mouse neurons by the mean of geometrical growth constraints, i.e. by the use of adhesive micro-patterns on siliconized glass substrates. Such a process thus excludes chemical guidance or specific adhesion mechanisms. This study explores two different types of geometrical constraints: Axons from the soma to the neurite tip are compelled to adopt the shape of isolated elastic beams, which model semiflexible polymers, the critical buckling load is enhanced when branched supports are included. Therefore, we conjecture that an optimal branching angle is found by looking at the competition between branching providing collective structural support, which results in polymerization of an axon with 39% of efficacy (N= 160 cells, 3 different cultures). The second one derives from the suggested relationship between neurite mechanical tension and axonal elongation, and is based on the design of wavy neurite’s shape. Its efficacy reach 0.51% (N= 300 cells, 3 different cultures). The combination of these two constraints into a final pattern yields an efficacy of 82% (N= 83 cells, 2 different cultures). These results not only provide an important tool for creating neural model networks but also point out an important role of intrinsic neurite tension during axon differentiation.

9:12AM A39.0007 Matrix rigidity optimizes the polarization of stem cells  
ASSAF ZEMEL, Institute of Dental Sciences, the Hebrew University-Hadassah Medical Center, Jerusalem, 91120, Israel, FLORIAN REHFELDT, Georg-August University, Ill. Physics Institute, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany, ANDRE BROWN, DENNIS DISCHER, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA, SAMUEL SAFRAN, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel — We present a theoretical model and experiments to explain the non-monotonic dependence of stress-fiber polarization in stem cells on matrix rigidity. The theory generalizes the treatment of elastic inclusions to “living” inclusions (cells) whose active polarizability, unlike non-living matter, depends on the feedback of cellular forces that develop in response to matrix stresses. We demonstrate experimentally that the stress fibers in adult mesenchymal stem cells, generally orient parallel to the long axis of the cells, with an anisotropy that depends non-monotonically on substrate stiffness. Consistent with these experiments, our theory predicts that the magnitude of the cellular force increases monotonically with the matrix rigidity while the polarization anisotropy shows a maximum that depends on the cell shape and the elastic modulus of the medium. These findings offer a mechanical correlate for the observation that stem cell differentiation optimizes in a range of matrix rigidities that depends on the tissue type.

9:24AM A39.0008 Structure at the Leading Edge  
D. A. QUINT, J. M. SCHWARZ, M. C. MARCHETTI, Syracuse University — The leading edge of a crawling cell is propelled forward by a polymerizing network of branched actin filaments. This emergent structural array seems to be rigid enough to support and push against the cell membrane within the appropriate time scales under which cell motility can be realized. We seek to understand the strategies different cell types use to generate the large force required to push cells through the extracellular matrix. We model the actin network as a collection of isolated elastic beams, which model semiflexible polymers, the critical buckling load is enhanced when branched supports are included. Therefore, we conjecture that an optimal branching angle is found by looking at the competition between branching providing collective structural support, which results in polymerization of an axon with 39% of efficacy (N= 160 cells, 3 different cultures). The second one derives from the suggested relationship between neurite mechanical tension and axonal elongation, and is based on the design of wavy neurite’s shape. Its efficacy reach 0.51% (N= 300 cells, 3 different cultures). The combination of these two constraints into a final pattern yields an efficacy of 82% (N= 83 cells, 2 different cultures). These results not only provide an important tool for creating neural model networks but also point out an important role of intrinsic neurite tension during axon differentiation.

9:36AM A39.0009 Chemotactic strategy of Vibrio alginolyticus studied with an optical trap  
SUDDHASHIL CHATOPADHYAY, TUBA ALTINDAL, XIE LI, XIA-LUN WU, University of Pittsburgh — The canonical "run" and "tumble" mode of chemotaxis, employed by multiple flagellated cells such as Escherichia coli, has been studied in great detail over the years. In this work we will demonstrate the usage of an optical trap for studying the chemotaxis of cells belonging to the single flagellated strain of Vibrio alginolyticus. This method allows precise and direct observation of chemotactic response, while the cell is exposed to various chemical signals (positive/negative gradient or no chemicals). We have studied the response of the flagellar motor with a precise control on the input signal (chemical gradient), such that a cell can be forced to move up or down a chemical gradient, a control which is not attainable for free swimming cells. The optical trap does not restrict the rotational motion of the bacterium and allows the state of the motor (clockwise or counter clockwise rotation) to be monitored continuously. Our group has recently observed an active flagellar movement (called the "flagellar flick") that is used by cells of Vibrio alginolyticus to reorient their direction of swimming. We consider this mode in addition to "back and forth" swimming employed by these cells. A modified chemotactic strategy is proposed and tested using the optical trap.

9:48AM A39.0010 Chemotaxis in Marine Bacterium Vibrio alginolyticus  
LI XIE, SUDDHASHIL CHATOPADHYAY, TUBA ALTINDAL, XIAO-LUN WU, University of Pittsburgh — We investigated swimming behavior of marine bacterium Vibrio alginolyticus in an uniform chemical environment. The typical bacterial trajectory consists of consecutive run (forward swimming) and reverse (backward swimming) intervals with occasional sudden changes of swimming directions, which we call "flagellar flicks". This mode of chemotaxis is different from the canonical run-and-tumble strategy adopted by Escherichia coli and monotonous-like in the bacterial swimming time series which results in the apparent turbulent dispersion. We measured the statistical distributions of run T_{run} and reverses T_{rev} time intervals, P(T_{run}) and P(T_{rev}), and found that while the back-swimming time appears to have a well-defined time scale of 0.5 s, the forward swimming time is more broadly distributed, suggestive of a Poisson process.

Measurements of the time interval T_{flick} between the consecutive directional changes show that P(T_{flick}) is also peaked at a finite time, T_{flick} ~ 1 s, and the mean directional change is ∆θ ~ 70°. Interestingly, this ∆θ observed is nearly optimal for efficient randomization of swimming directions. Altogether, our experiments suggest that V. alginolyticus employs both run-and-reverse and flicking activities for chemotaxis, and this behavior presumably optimizes their foraging efficiency in a turbulent environment.
The flagellar “flick”: direction randomization in single flagellated cells of V. alginolyticus

Follow a “back” and “forth” swimming pattern. Inspired by the observation that V. alginolyticus cells were able to rapidly accumulate around a point source of a chemoeffectant, we have identified a previously unknown mechanism in which an active movement of the flagellum is used to randomize the swimming direction. Fluorescently labelled cells clearly demonstrated that bending of the flagellum is responsible for imparting direction changes to the cell body. Clues obtained from high speed video, bright-field microscopy and fluorescent imaging suggest a series of steps involved in the flagellar “flick”. An investigation of the energetics of the proposed mechanism leads to the conclusion that the directional change may be connected to the flagellar motor, which normally propels the cell body.

10:12AM A39.00012 Probing the Dynamics of Cellular Traction Forces with Magnetic Micropost Arrays

CORNELIA KRAMER, Johns Hopkins University, CHRISTOPHER CHEN, University of Pennsylvania, DANIEL REICH, Johns Hopkins University — Mechanical forces on living cells are associated with changes in cellular function. For example, vascular smooth muscle cells are known to undergo a mechanical feedback response to increased stress, which can result in atherosclerosis. We have recently developed a magnetic micropost array, a novel device for measuring cellular traction forces that simultaneously enables the application of localized external forces to cells. The device consists of an array of micrometer scale holes, each of which can be selectively actuated by a micromagnet. Forces are applied to the adherent cell via a magnetic torque on a cobalt nanowire embedded in a single post. Initial results showed an active and non-local cellular response to applied forces in mouse fibroblast cells. We will present results on the spatially resolved dynamics of traction forces exerted by smooth muscle cells over time in response to constant and time-varying stimulation. The observation of biochemical and mechanical regulation of the subcellular redistribution of force may allow insights into cellular mechanotransduction and control of cell function.

10:24AM A39.00013 Differential cellular response to linear and strain-stiffening hydrogel substrates

JESSAMINE P. WINER, SHAHNA A. OAKE, BETHANY C. BAUMANN, PAUL A. JANMEY, University of Pennsylvania — Many cell types act as tensometers, modulating their spread area, motility, and protein expression in response to the substrate stiffness. Studies of stiffness sensing typically employ linear elastic materials whose stiffness is independent of the applied strain. Biological gels, however, often stiffen in response to increasing strain. Fibroblasts and mesenchymal stem cells adherent to linearly elastic gels typically display a small, round phenotype on soft substrates and increase spread area as the elastic modulus of their substrate increases. On the strain-stiffening biopolymer gel fibrin, the same cell types are maximally spread even when the gel’s low strain elastic modulus would predict a round morphology. Traction microscopy reveals that cells apply active displacements of several microns up to five cell lengths away, and atomic force microscopy shows that these displacements locally stiffen the gel by deforming it beyond its linear range. The magnitude of cell-applied strains is inversely related to the gel’s low strain elastic modulus and results in long distance cell-cell communication and alignment.


S. BAILEY, Department of Physics, The Ohio State University, J. GUMP, Naval Surface Warfare Center, Indian Head, MD, R. SOORYAKUMAR, C. JAYAPRAKASH, Department of Physics, The Ohio State University, M.S. VENKITESHWAR, M. BULLMORE, Department of Optometry, The Ohio State University, M. TWA, College of Optometry, University of Houston — Focusing the eye on a near object results in an increase in its optical power brought about by contraction of the ciliary muscles and an increase in the lens surface curvature. Distant vision occurs when the muscular force flattens the lens. Central to the ability of the lens to alter shape are its mechanical properties. Thus, given that hardening of the lens would impede deformation and reduce its ability to undergo the changes required for accommodation, a noninvasive approach to measure the elastic properties of the lens is valuable. We present results of Brillouin scattering from bovine and human lenses (from the organ donor program at The Ohio State University) that measure their high frequency acoustic response. These measurements are conducted with a few milli-watts of laser power and, in the case of bovine lenses, from entire intact eye globes, allow the stiffness of scattering from bovine and human lenses (from the organ donor program at The Ohio State University) that measure their high frequency acoustic response. The results will be compared to values of the shear- and bulk-moduli determined from other techniques and the implications of differences in these moduli discussed.

10:48AM A39.00015 Physical Description of Mitotic Spindle Orientation During Cell Division

ANDREA JIMÉNEZ-DALMARONI, University College London, UK, MANUEL THÉRY, Laboratoire Biopuces CEA, Grenoble, France, VICTOR RACINE, MICHEL BORNENS, Institut Curie, Paris, France, FRANK JÜLICHER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — During cell division, the duplicated chromosomes are physically separated by the action of the mitotic spindle. The spindle is a dynamic structure of the cytoskeleton, which consists of two microtubule asters. Its orientation defines the axis along which the cell divides. Recent experiments show that the spindle orientation depends on the spatial distribution of cell adhesion sites. Here we show that the experimentally observed spindle orientation can be understood as the result of the action of cortical force generators acting on the spindle. We assume that the local activity of force generators is controlled by the spatial distribution of cell adhesion sites determined by the particular geometry of the adhesive substrate. We develop a simple physical description of the spindle mechanics, which allows us to calculate the torque acting on the spindle, as well as the energy profile and the angular distribution of spindle orientation. Our model accounts for the preferred spindle orientation, as well as the full shape of the angular distributions of spindle orientation observed in a large variety of pattern geometries. M. Théry, A. Jiménez-Dalmaroni, et al., Nature 447, 493 (2007).
8:12AM A40.00002 Structural and functional allostery wiring diagrams in GroEL/GroES1. RIINA TEHVER, JIE CHEN, D. THIRUMALAI, University of Maryland — Repeated cycling between distinct allosteric states is required for the functions of numerous biological nanomachines. Determining the specific residues that are responsible for transmitting allosteric signals is needed to understand their operation. Using structural perturbation analysis and evolutionary correlations of mutations of residues, we determine networks of key residues in molecular chaperonin GroEL and its cochaperonin GroES. GroEL is a molecular machine that rescues aggregation-prone misfolded proteins. Its functional cycle consists of a series of large-scale allosteric transitions between the T, R, R' and R'' states. The corresponding structural rearrangements facilitate substrate protein capture, refolding, and release. The networks of residues we find provide a microscopic foundation for the cooperativity of the allosteric transitions and a linkage between substrate protein binding and ATPase activity of GroEL.

1 RT is a National Institute of General Medical Sciences postdoctoral fellow (1F32GM082009). DT is grateful to the NIH (1R01GM067851-01) and the AF Office of Scientific Research (FA9550-07-1-0098).

8:24AM A40.00003 Decoupling of Protein Dynamics from the Solvent Viscosity. SHEILA KHODADADI, Department of Polymer Science, The University of Akron, ARMISTEAD KATHLEEN, University of Kansas, ALEXEI SOKOLOV, Department of Polymer Science, The University of Akron — Studies show that solvent viscosity has a strong influence on protein dynamics and activity, but the detailed mechanism of the solvent-protein interactions is not fully understood. Using dielectric spectroscopy we were able to identify a protein related relaxation process of myoglobin in water-glycerol and water-sucrose solutions. We demonstrate that the rate of biochemical reaction (taken from literature1) follows the protein related relaxation observed in dielectric spectra. Also our results reveal decoupling of the protein dynamics from solvent viscosity. This finding explains the known in literature decoupling of protein activity from solvent viscosity and demonstrates direct connection between protein dynamics and its functionality. Possible microscopic mechanisms of this decoupling are discussed at the end. 1. Kleinert, T.; et al. Biochemistry 1998, 37, 717.

8:36AM A40.00004 Phosphorylation of histone H3 Thr 118 converts nucleosomes into a higher-mass complex1. JUSTIN NORTH, MICHAEL POIRIER, Department of Physics, The Ohio State University, MICHELLE FERDINAND, JENNIFER OTTESEN, Department of Biochemistry, The Ohio State University — The nucleosome is the fundamental unit of DNA compaction in eukaryotes by which 147 base pairs of DNA wrap 1.7 times around a protein complex called the histone octamer. Numerous chemical modifications are found in vivo that alter octamer surface charge and shape. One such modification is phosphorylation of histone H3 residue Thr 118 located in the dyad region of the nucleosome. We find that phosphorylated H3 T118 (H3 pT118) octamer, when reconstituted with DNA of about 200bp, suppresses nucleosome formation and promotes formation of a higher-mass DNA-protein complex. Coordinateophorically, dephosphorylation of H3 pT118 octamer by phosphatase results in reconstitution of normal nucleosomes. DNase I footprinting reveals that while DNA contacting the octamer surface in nucleosomes is less accessible than free DNA, the entire DNA strand is equally accessible in the higher-mass complex and is digested at one-third the rate of free DNA.

1 This work was supported by the Burroughs Wellcome Career Award in Basic Biomedical Sciences and NIH grant No. R01 GM083055

8:48AM A40.00005 The Role of gp120 Flexibility in Binding. A.J. RADER, Indiana University-Purdue University Indianapolis — Current treatment of the human immunodeficiency virus (HIV) focuses on delivering several drugs to to a few specific viral protein targets. A complementary antiviral therapy involves targeting the process of viral entry. Viral entry is a dynamic process which involves a series of conformational changes by the HIV envelope glycoproteins (gp120 and gp41). The extraordinary conformational flexibility, glycosylation and strain variability of these proteins complicate the development of an effective vaccine. We present results from the graph theoretical analysis of flexibility and rigidity using the Floppy Inclusion and Rigid Substructure Topography (FIRST) software for all known HIV-1 gp120 structures. Comparisons between structures using this mechanical stability and intrinsic flexibility is used to identify a consensus rigid region that might serve as drug targets in a pre-complex conformation. Furthermore, analysis of structures with various binding partners illustrates the differential partitioning of mechanical flexibility and strain. We relate these differences in mechanical stability to thermodynamic differences in binding and stabilizing mutations.

9:00AM A40.00006 AP helical stability in salt solutions. ELIANA ASCIUTTO, Duquesne University, KAN XIONG, University of Pittsburgh, SANFORD ASHER, University of Pittsburgh, JEFFRY MADURA, Duquesne University — Protein dynamics depends on the environment and the inclusion of salts in the simulation of folding/unfolding becomes extremely necessary when comparing energy barriers or reaction rates with experimental results. The aim of this study is to investigate the effects of three sodium salts: NaClO4, NaCl and Na2SO4 on the helical stability of AP, a mainly alanine peptide. The dependence of the peptide helical stability on the environment has been studied using Replica Exchange Molecular Dynamics (REMD) simulations, Circular Dichroism (CD) and Ultraviolet Raman Resonance Spectroscopy (UVRS) experiments. It was found that NaClO4 solution strongly stabilizes the helical states and that the order in which sodium salts stabilize the peptide helical states follows a reverse Hofmeister Series (ClO4−<Cl−<SO42−). Another interesting result found is that ClO4− ions are attracted to the backbone; Cl− ions are repelled while SO42− ions are attracted to the positive side chains. A thorough investigation of the ion effects on the first and second solvation water along with the Kirkwood-Buff theory for solutions allowed us to explain the physical mechanisms involved in the observed ion specific effects.

9:12AM A40.00007 Computational modeling of protein folding assistance by the eukaryotic chaperonin CCT. MANORI JAYASINGHE, GEORGE STAN, University of Cincinnati — Chaperonins are biological nanomachines that promote protein folding using energy derived from ATP hydrolysis. Structurally, chaperonins are large oligomeric complexes that form double-ring construct, enclosing a central cavity that serves as folding chamber. Our focus is on the substrate binding mechanisms of the Eukaryotic chaperonin CCT and Archaeal chaperonin Thermosome. We contrast our results with the annealing action of the bacterial chaperonin GroEL of E. coli, currently the best studied for chaperonin machinery. CCT was suggested to be more selective towards the substrate recognition where as GroEL is more promiscuous due to the hydrophobic interactions. We study the interaction of CCT with Tubulin, one of its stringent substrates. Using molecular docking and molecular dynamics simulations, we probe binding of a βtubulin peptide (205-274) to the CCTβ apical domain. We identify a versatile binding mechanism, involving mostly hydrophobic interactions with the helical region and electrostatic interactions with the helical protrusion region. This specific substrate-protein recognition mechanism is likely to be optimized for specific substrate protein-CCT subunit pairs.

1 American Heart Association
Substrate protein recognition mechanism of archaenal and eukaryotic chaperonins. Chaperonins are double ring-shaped biological nanomachines that assist protein folding. Spectacular conformational changes take place within each chaperonin ring using energy derived from ATP hydrolysis. These changes result in transitions from the open to the closed ring. Substrate proteins bind to the open ring and are encapsulated within the closed ring cavity. We focus on the substrate protein recognition mechanism of archaenal and eukaryotic chaperonins. We predict substrate protein binding sites using structural and bioinformatic analyses of functional states during the chaperonin cycle. Based on large changes in solvent accessible surface area and contact maps we glean the functional role of chaperonin amino acids. During the transition between open to closed chaperonin ring, the largest change in accessible surface area of amino acids is found in helical protrusion and two helices located at the cavity opening. Our calculations suggest that the helical protrusion and two helices constitute the substrate protein binding site.

Supported by NSF under grant no. MCB-0744077. American Heart Association
At very low temperatures, we simulate the Kondo lattice model with the continuous-time quantum Monte Carlo method recently developed by one of the authors to developed an exact description of heavy fermion materials. We propose a layered Kondo lattice model for the quantum critical superconductor $\beta$-YbAlB$_4$, and we examine the effects of antiferromagnetic interactions on the composite pairing. If both gaps are d-wave, they couple linearly, mutually enhancing the superconducting transition temperature.

**Monday, March 16, 2009 8:00AM - 10:24AM**

**Session A41 DMP: Heavy Fermions 413**

8:00AM A41.00001 Realistic simulation of Kondo lattice model: application to Ce compounds, MUNEISHI MATSUMOTO, MYUNG JOON HAN, UC Davis, JUNYA OTSUKI, Tohoku University, Japan, SERGEY SAVRASOV, UC Davis — In order to do a good description of heavy fermion materials at very low temperatures, we simulate the Kondo lattice model with the continuous-time quantum Monte Carlo method recently developed by one of the authors combined with the conduction-electron density of states given by first-principle calculations and performing self consistency using dynamical mean field theory. We discuss our results for Ce compounds down to the temperature range of $O(1)$ K using realistic values of crystal-field and spin-orbit level splitting.

8:12AM A41.00002 Layered Kondo lattice model for quantum critical superconductor $\beta$-YbAlB$_4$, ANDRIY NEVIDOMSKYY, PIERS COLEMAN, Rutgers University — We perform a theoretical analysis of the magnetic and electronic properties of the quantum critical heavy fermion superconductor $\beta$-YbAlB$_4$. Using a combination of the realistic material modelling and single-ion crystal field analysis, we propose a layered Kondo lattice model for this system, in which two dimensional boron layers are Kondo-coupled via interlayer Yb moments in a $J_g = \pm 5/2$ state. This model fits the measured single ion magnetic susceptibility and predicts a substantial change in the electronic anisotropy as the system is pressure-tuned through the quantum critical point. An interesting connection is made between this model and the Kondo effect in Coulomb-blockaded quantum dots. We also calculate the Fermi surface and the angular dependence of the extremal orbits relevant to the de Haas-van Alphen measurements.

8:24AM A41.00003 Interplay of Composite Pairs and Magnetism in Heavy Fermion Superconductors, REBECCA FLINT, PIERS COLEMAN, Rutgers University — Superconductivity in PuMg$_{2x}$, $M = \{Co, Rh\}$ and NpPd$_2$Al$_2$ can be treated within a two channel Kondo lattice model, where the electron-spin scattering develops an Andreev component, creating a composite bound state of a spin-flip and a pair of electrons. We extend this model to CeMn$_2$, where magnetism and superconductivity exist in close proximity by including antiferromagnetic interactions. Different crystal symmetries lead to composite pairing with either a g-wave gap or d-wave gap, while antiferromagnetism leads to RVB superconductivity with a d-wave gap. Within a symplectic large $N$ limit, we examine the effects of antiferromagnetic interactions on the composite pairing. If both gaps are d-wave, they couple linearly, mutually enhancing the superconducting transition temperature.

8:36AM A41.00004 Very low temperature specific heat and magnetoresistance of PrOs$_x$Sb$_{12}$, BOHDAN ANDRAKOA, University of Florida — Heavy fermion character of PrOs$_x$Sb$_{12}$ has been concluded based on its superconducting properties, such as large values of the discontinuity $C$ and upper critical field slope at $T_c (1.85$ K). On the other hand, normal state properties do not provide any strong evidence of the heavy fermion behavior. In particular, $m^*$ enhancement measured by the de Haas van Alphen technique in overcritical fields and below 700 mK is typical of transition metals, suggesting that the heavy fermion state is either suppressed by magnetic fields or collapses at low temperatures. We reexamine these possible scenarios using new magnetoresistance and specific heat, down to 50 mK, data.

8:48AM A41.00005 Effect of ferromagnetism on unconventional superconductivity in the Pr$_{1-x}$Nd$_x$Os$_8$Sb$_{12}$ system, P.-C. HO, Physics/CSU-Fresno, M. B. MAPLE, T. YANAGISAWA, W. M. YUHASZ, N. P. BUTCH, A. A. DOORAGHI, C. C. ROBINSON, Physics/UCSD — The filled skutterudite compound PrOs$_8$Sb$_{12}$ is a 1.85 K heavy fermion superconductor (SC), which displays unconventional SC property, such as existence of multiple SC phases and point nodes in the SC energy gap and the appearance of internal magnetic field in its SC state. NdOs$_8$Sb$_{12}$ is a mean-field type magnet with a low Curie temperature $\sim 1$ K. The Nd substitution in the Pr$_{1-x}$Nd$_x$Os$_8$Sb$_{12}$ system has been carried out in order to investigate the ferromagnetic (FM) effect on the unconventional SC of PrOs$_8$Sb$_{12}$ and the quantum critical behavior in this system. SC state in this system disappears near $x \sim 0.55$ and FM extends into the SC region. The $x$ dependence of the 0-K extrapolated upper critical field $H_{c2}(x, T = 0)$ has curvature breaking at $x \sim 0.3$. The $H_{c2}(x, T = 0)$ data can be analyzed by multiple pair breaking effect due to magnetic field, appearance of impurity, and the exchange field generated by magnetic ions. However, when $H_{c2}(x, T = 0)$ of Pr$_{1-x}$Nd$_x$Os$_8$Sb$_{12}$ is compared to that of a BCS SC La$_{3-x}$Gd$_x$In, the curvature in the regime where $x/x_{cr} < 0.5$ is significantly different. Detail analysis and comparison will be discussed. Research at CSU-Fresno supported by RC CCSA #7669 and Fresno State start-up fund; at UCSD by US DOE and NSF; at Hokkaido U by MEXT, Japan.

9:00AM A41.00006 The role of $\beta$-electrons at the Fermi surface of the heavy fermion superconductor $\beta$-YbAlB$_4$, EOEIN O’FARRELL, D.A. TOMPSEET, S.E. SEBASTIAN, Cavendish Laboratory, University of Cambridge, N. HARRISON, NHMFL, MS-ES36, Los Alamos National Laboratory, C. CAPAN, Department of Physics and Astronomy, University of California, Irvine, L. BALICAS, NHMFL, Tallahassee, K. KUGA, T. MATSUO, M. TOMONAGA, S. NAKATSUI, ISSP, University of Tokyo, G. CSÁNYI, Department of Engineering, University of Cambridge, Z. FISK, Department of Physics and Astronomy, University of California, Irvine, M.L. SUTHERLAND, Cavendish Laboratory, University of Cambridge — We present a detailed quantum oscillation study of the Fermi surface of the recently discovered Yb-based heavy fermion superconductor $\beta$-YbAlB$_4$. We compare the data, obtained at fields from 10 to 45 Tesla, to band structure calculations performed using the local density approximation. Analysis of the data suggests that the $\beta$-electrons are delocalized and contribute to the fermi volume at all fields. We comment on the significance of these findings for the observed quantum critical and superconducting properties of this material.

The electronic structure of PuCoGa$_5$ and PuSb$_2$ is anisotropic and probably has a paramagnetic effect under field along the $c$-axis because of the divergent behavior of the Ising like $c$-axis susceptibility. Moreover, the coherence maximum around 11 K, which defines the depth of the Kondo effect, is observed.

These results suggest that pressure increasing causes the suppressing of Kondo effect in YbB$_2$. The Kondo effect and the pressure dependence of Debye temperature as $\langle D/P \rangle = (1.46 \pm 0.30)$ K/GPa which is calculated using Bloch-Gr"uneisen approximation. Measurements of the temperature dependent $\gamma$-spin-lattice relaxation rate $1/T_1$ show an increasing rate for decreasing temperature ($T > 50$ K), followed by a broad maximum near 30 K. These results are discussed in light of the heavy-fermion like nature of the material.

Supported by NSF Materials World Network grant DMR-0710525.

9:12AM A41.00007 Superconducting Properties of the Non-Fermi-Liquid System $\beta$-YbAlB$_4$. KENTARO KUGA, YOSHITOMO KARAKI, YOSUKE MATSUMOTO, YÔ MACHIDA, NAOKI HORIE, SATORU NAKATSUJI, Institute for Solid State Physics

9:24AM A41.00008 Electronic Structure of PuCoGa$_5$ and PuSb$_2$ Using Angle-Resolved Photoemission. [1] J.J. JOYCE, Los Alamos National Laboratory, T. DURAKIEWICZ, K.S. GRAHAM, D.P. MOORE, J.M. WILLS, JIAN-XIN ZHU, E.D. BAUER, J. MITCHELL — The electronic structure of PuCoGa$_5$ and PuSb$_2$ is investigated using angle-resolved photoemission (ARPES). Details of the sharp quasiparticle peak at the Fermi energy are presented giving insight into the details of the mechanisms which give rise to strongly correlated characteristics in these materials. Additionally, the details of the dual nature of the 5f electrons are explored via characterization of more localized 5f states well removed from the Fermi energy. The ARPES data is compared with electronic structure models which move beyond the density functional theory approach to address the strong electron correlations present in Pu compounds as well as the dual nature of the 5f electrons.

supported by USDOE BES and LANL LDRD.

9:36AM A41.00009 $^7$Li NMR Study of Yb$_2$LiGe$_4$: A Possible Kondo Insulator. [1] M. J. GRAF, V. LANIO, Dept. of Physics, Boston College, Chestnut Hill, MA 02467, USA, P. CARRETTA, Dept. of Physics A. Volta, Univ. of Pavia, 27100 Pavia, Italy, YU. GRIN, S. PETER, Max-Planck-Institut fur Chemische Physik fester Stoffe, 01187 Dresden, Germany — We report on the temperature-dependent resistivity, magnetic susceptibility, and nuclear spin-lattice relaxation rate of polycrystalline Yb$_2$LiGe$_4$. The parent compound, Yb$_3$Ge$_4$, is known to be mixed valent. The increasing susceptibility and resistivity with decreasing temperature are consistent with a Kondo insulator. Measurements of the temperature dependent $^7$Li-spin-lattice relaxation rate $1/T_1$ show an increasing rate for decreasing temperature ($T > 50$ K), followed by a broad maximum near 30 K. These results are discussed in light of the heavy-fermion-like nature of the material.

Work supported by NSF Materials World Network grant DMR-0710525.

9:48AM A41.00010 Revealing the Ce gamma-alpha Isostructural Phase Transition. [1] YI WANG, LOUISE HECTOR, SHUNLI SHANG, LONG-QING CHEN, ZI-KUI LIU, PENN STATE TEAM, GM COLLABORATION — Since its discovery eighty years ago, the gamma-alpha iso-structural phase transition in cerium has been the subject of numerous theoretical studies. Existing theories, however, yield inaccurate results. Nowhere is this more evident than with the 50-200% disagreement between existing theoretical predictions of the critical point and experiment. We resolve this issue by explicitly incorporating finite temperature mixing of the Ce nonmagnetic and magnetic states into a novel partition function wherein all input quantities are computed with density functional theory. Unique to our approach is the calculation of vibrational properties from phonon theory. The critical behavior of the transition is shown to be controlled by the configurational mixing entropy between the magnetic and nonmagnetic states. Our theoretical framework leads to predicted values of the critical point and equation-of-state that are in remarkably close agreement with experiment and thereby places the Ce gamma-alpha phase transition on a firm theoretical foundation.

10:00AM A41.00012 ABSTRACT WITHDRAWN.

10:12AM A41.00011 Pressure Effect on The Kondo Behavior of Layered YbB$_2$. [1] BORA KALKAN, Advanced Materials Research Group, Physics Department, Hacettepe University, Ankara 06800, Turkey — The structural properties and the effect of pressure on the electrical properties of polycrystalline YbB$_2$ were investigated via x-ray diffraction and x-ray photoemission spectroscopy (XPS) under ambient pressure and resistivity measurements up to 6.2 GPa. Rietveld refinement confirmed the hexagonal layered structure of YbB$_2$ in P6/mmm space group with $a=b=3.2522(2)$ Å and $c=3.7297(4)$ Å lattice parameters. XPS and low temperature measurements proved the magnetically ordered ground state of YbB$_2$ in which Yb ion has already magnetic trivalent state under ambient pressure. $\rho(T)$ measurements down to 3.5 K at various pressures exhibit a typical Kondo lattice behavior at low temperatures with a resistivity minimum around 23 K and a coherence maximum around 11 K, which define the depth of the Kondo effect. Moreover, resistivity results yield the gradual weakening of the contribution of Kondo effect and the pressure dependence of Debye temperature as $\langle d\rho/T \rangle = (1.46 \pm 0.30)$ K/GPa which is calculated using Bloch-Gr"uneisen approximation. These results suggest that pressure increasing causes the suppressing of Kondo effect in YbB$_2$.


11:15AM B1.00001 Graphene and its chemical derivatives. [1] KOSTYA NOVOSELOV, University of Manchester — Graphene is a first two-dimensional atomic crystal. In my talk I’ll overview our latest results on the electronic properties of graphene, and discuss a possibility of band structure engineering by chemical modification of this material.
11:51AM B1.00002 The high-field state at the Dirac Point in graphene\(^1\), N. PHUAN ONG\(^2\), Princeton University — The discovery of the quantum Hall Effect in graphene has generated considerable interest in the state at the Dirac Point in a magnetic field \(H\). In intense \(H\), the 4-fold degeneracy of the \(n = 0\) Landau Level (LL) is lifted by the enhanced exchange energy. Among the broken symmetry states proposed are the quantum Hall ferromagnet, the quantum Hall insulator state, excitonic condensation, and charge-density-wave formation. A subset of these theories propose counter-propagating edge states that remain conducting in large \(H\). We have performed measurements of the resistance \(R_{xx}\) and Hall resistance \(R_{xy}\) to fields of 33 T at temperatures \(T\) from 0.3 to 50 K in \ (~6) graphene samples. We find that, as \(T\) decreases below 10 K, \(R_0 = (= R_{xx} \text{ at the Dirac Point})\) undergoes a steep increase with a divergence consistent with a field-driven transition to an insulating high-field state. The divergence in \(R_0\) fits well to the Kosterlitz-Thouless (KT) form \(\exp[\sqrt{h/(\hbar - T)}]\) with \(h = H/H_c\) and \(b \sim 1.4\). The critical field \(H_c\) is sample dependent (12 T to 33 T ), and correlates with the disorder as measured by the offset gate voltage \(V_0\) and the zero-\(H\) mobility. The divergence in \(R_0\) is strictly confined to the \(n = 0\) LL (bracketed by the sublevels \(\nu = \pm 1\)). The peaks with \(n = \pm 1\) remain near the values \(h/e^2\). Using an ultralow-power (3 kW), voltage-regulated technique, we show that the KT-fit to \(R_0\) is valid over 3 decades (40 kΩ to 40 MΩ). The steepness of the \(R_0\) vs. \(T\) curves implies a bulk gap \(\Delta\) of magnitude 15-20 K that decreases when \(H\) falls below \(H_c\). We compare our findings with the various proposed models. We will also report thermopower and Nernst measurements taken to fields of 14 T.

\(^1\)Supported by NSF Grant DMR-0819860. High-field experiments were performed at the National High Magnetic Field Lab., Tallahassee.

\(^2\)co-authors: J. G. Checkelsky and Lu Li

12:27PM B1.00003 Quantum Carrier Collimation in Locally Gated Graphene Heterojunction Devices, PHILIP KIM, Columbia University — While electron optics such as lensing and focusing have been demonstrated experimentally, building a collimated electron interferometer in two unconfined dimensions has remained a challenge due to the difficulty of creating electrostatic barriers that are sharp on the order of the electron wavelength. Owing to the suppression of backscattering experienced by the chiral quasiparticles, graphene provides an ideal medium to realize the quantum engineering of electron wave functions. In this presentation, we show our progresses in wave function engineering in graphene devices by demonstrating the conductance oscillations in extremely narrow graphene heterostructures where a resonant cavity is formed between two electrostatically created bipolar junctions. Analysis of the oscillations confirms that bipolar heterojunctions have a collimating effect on ballistically transmitted carriers. The robustness of the oscillatory conductance to scattering provides a novel probe of the ballistic physics of graphene at the Dirac point and makes graphene heterojunctions a promising tool for the coherent manipulation of carriers in mesoscopic systems.

1:03PM B1.00004 Robustness of quantum Hall effect in locally gated graphene devices, DMITRY ABANIN, Princeton University — Two-terminal conductance of locally gated graphene p-n-p heterojunctions in the quantum Hall regime is quantized at integer and fractional values, owing to the edge states equilibration. We study the sensitivity of this quantization to finite longitudinal conductivity in the locally gated inner region of the junction. Taking a bulk conductivity approach, we solve spatially non-uniform conduction problem exactly by a conformal mapping method. We find that the robustness of the conductance quantization strongly depends on the geometry of the locally gated region, as well as on the densities in the inner and outer regions. We present a detailed comparison of our predictions with recent experimental data, finding good agreement.

1:39PM B1.00005 Octet Quantum Hall Effect in Graphene Bilayers\(^1\), ALLAN H. MACDONALD, University of Texas at Austin — Interaction driven integer quantum Hall effects are anticipated [1]in graphene bilayers because of the near-degeneracy of eight Landau levels which appear near the neutral system Fermi level at filling factors between \(\nu = -4\) and \(\nu = 4\). The bilayer graphene octet exhibits a wide variety of broken symmetry states, with Ising, XY and Heisenberg character which can be controlled by an external field which creates an electric potential difference between the two layers. Because of the peculiarities of the bilayer graphene electronic structure states with \(n=0\) and \(n=1\) orbital character are degenerate. I will explain predictions that an intra-Landau-level cyclotron resonance signal will appear at some odd-integer filling factors, accompanied by collective modes which are nearly gapless and have approximate k\(^{3/2}\) dispersion. This talk will be based on work performed in collaboration with Yafis Barlas, Rene Cote, Kentaro Nomura, and Jules Lambert.


\(^1\)Supported by NSERC, by the Welch Foundation, and by the NSF under grant DMR-006489.

Monday, March 16, 2009 11:15AM - 2:15PM —
Session B2 DCMP: HTSC: Fermi Pockets and Quantum Oscillations

11:15AM B2.00001 Competing order, Fermi surface reconstruction, and quantum oscillations in high temperature superconductors\(^1\), SUDIP CHAKRAVARTY, UCLA — Recent quantum oscillation measurements in underdoped high temperature superconductors in high magnetic fields and low temperatures have ushered in a new era. These experiments appear to explore the normal state from which superconductivity arises and provide evidence of a reconstructed Fermi surface consisting of electron and hole pockets in a regime in which such a possibility was previously considered to be remote. Here we explain the observations with the theory that the alleged normal state exhibits a hidden order, the \(d\)-density wave. The success of our analysis underscores the importance of spontaneous breaking of symmetries, Fermi surface reconstruction, and quasiparticles. We primarily focus on the version of the order that is commensurate with the underlying crystalline lattice, but also touch upon the consequence of incommensuration. In addition, the effect of possible bilayer splitting and the nature of quantum oscillations in the mixed state are addressed.

\(^1\)Supported by NSF DMR-0705092

11:51AM B2.00002 Quantum Oscillations in underdoped YBCO: the nature of Fermi surface reconstruction and evolution toward the Mott insulating regime, SUCHITRA SEBASTIAN, Cambridge University — I will present results of quantum oscillation measurements we have measured in underdoped YBCO_{1+x} that reveal a small Fermi surface. Results of angular dependent measurements enable us to obtain clues as to the nature of order that reconstructs the Fermi surface. I will also present results of doping-dependent measurements that enable us to trace Fermi surface evolution as the insulating regime is approached. Work was performed in collaboration with N. Harrison, G. G. Lonzarich, C. Mielke, R. Liang, D. Bonn and W. Hardy
expected recovery of the usual Fermi-liquid metal on the high doping side is fundamental but ill understood. Here we uncover a new transformation in an 

natural tuning parameter that takes copper oxides from the antiferromagnet through the superconducting ‘dome’-shaped region. In the metallic state above 

This work was carried out in collaboration with Hongbo Yang, Jon Rameau, Tonica Valla, Alexei Tsvelik and Genda Gu and was supported by the Department of 

energy

immediate vicinity of the Fermi level is not particle-hole symmetric in the pseudogap phase. This is clear evidence that superconducting pairing does not originate 

from the Fermi arcs. The observations are also consistent with the possibility that the Fermi arcs are in fact the inner surface of the predicted Fermi pockets. 

This work was carried out in collaboration with Hongbo Yang, Jon Rameau, Tonica Valla, Alexei Tsvelik and Genda Gu and was supported by the Department 

of Energy.

1:03PM B2.00004 Field-Induced Quantum Critical Route to a Fermi Liquid in Overdoped 

(1)

Tl2Ba2CuO6+δ/2. TAKASADA SHIBAUCHI, Department of Physics, Kyoto University — In high temperature superconductivity, charge doping is a 

natural tuning parameter that takes copper oxides from the antiferromagnet through the superconducting ‘dome’-shaped region. In the metallic state above 

Tc, the standard Landau’s Fermi-liquid theory of metals, as typified by the temperature squared (AT2) dependence of resistivity, appears to break down. 

The expected recovery of the usual Fermi-liquid metal on the high doping side is fundamental but ill understood. Here we uncover a new transformation in an 

overdoped superconducting copper oxide Tl2Ba2CuO6+δ/2 from the non-Fermi to a Fermi-liquid ground state driven by magnetic field [1]. From the c-axis resistivity 

measured up to 45 T, we show that the Fermi-liquid AT2 features, accompanied by a field-linear magnetoresistance, appear above a field HFL. This crossover 

HFL decreases linearly with decreasing temperature T and lands at a quantum critical point (QCP) near the upper critical field Hc2(0). The Fermi-liquid 

coefficient A(II) shows a power-law diverging behavior on the approach to the QCP, indicating the second-order quantum phase transition at this field. 

The connection between the field-induced QCP and the pseudogap observed in the underdoped regime will be discussed.


1:39PM B2.00005 Fermi surface reconstruction in high-Tc superconductors , LOUIS TAILLEFER, University of Sherbrooke and Canadian Institute for Advanced Research — The recent observation of quantum oscillations in overdoped high-Tc superconductors (1), combined with their negative Hall coefficient at low temperature (2), reveals that the Fermi surface of hole-doped cuprates includes a small electron pocket. This strongly suggests that the large hole Fermi surface characteristic of the overdoped regime undergoes a reconstruction caused by the onset of some order which breaks translational symmetry. Here we consider the possibility that this order is “stripe” order, a form of combined charge / spin modulation observed most clearly in materials like Eu- doped and Nd-doped LSCO. In these materials, the onset of stripe order coincides with major changes in transport properties (3), providing strong evidence that stripe order is indeed the cause of Fermi-surface reconstruction. We identify the critical doping where this reconstruction occurs and show that the temperature dependence of transport coefficients at that doping is typical of metals at a quantum critical point (4). We discuss an 

interpretation of the pseudogap as a fluctuating precursor of the stripe-ordered phase.

This work was performed in collaboration with L. Balicas, D.A. Bonn, J. Chang, O. Cyr-Choinière, R. Daou, N. Doiron- Leyraud, W.N. Hardy, N.E. 


(2) D. LeBoeuf et al., Nature 450, 533 (2007).


Monday, March 16, 2009 11:15AM - 2:15PM — 

Session B3 FEd: 10,000 Undergraduate Physics Majors: Progress on Doubling 301/302

11:15AM B3.00001 Why Do We Need 10,000 Physics Majors?, THEODORE HODAPP, American Physical Society — The early 1960’s saw a huge increase in the number of physics majors, reaching an all time peak of just over 6000 per year. While the number plummeted in the next four decades, it has finally experienced a resurgence to nearly this number. The American Physical Society along with the American Association of Physics Teachers recently endorsed a call to double the number of undergraduate physics majors over the next decade. The main focus of this effort is to increase both the number of high school physics teachers and the fraction of women and under-represented minorities studying physics. In addition, a physics degree prepares an undergraduate with excellent skills that will serve her or him for a variety of occupations both in the sciences and in other fields. This talk will explore some of the data on physics majors and the rationale for taking the bold step of suggesting we try and educate 10,000 majors each year. Sputnik helped catalyze the nation 50 years ago – What is the Sputnik of today? Bring your thoughts and questions... we hope for a lively discussion.

11:51AM B3.00002 Successful Minority PhD Producing Programs – Bell Laboratories and the Meyerhoff Scholarship Program at UMBC, ANTHONY JOHNSON, University of Maryland Baltimore County — The Bell Labs Cooperative Research Fellowship Program for Minorities (CRFP), founded in 1972 was one of the first programs of its kind in the US to address the issue of under-representation of minorities in the fields of engineering, mathematics and science. As of 2000, well over 100 Ph.Ds graduated with CRFP sponsorship and a significant fraction joined the research ranks of Bell Labs. In the early days of the program as much as 50% of African American PhDs in Physics in the US were granted to students supported by CRFP. Another unique program initiated by Bell Labs in 1974 that introduced undergraduate students to cutting edge research was the Summer Research Program for Minorities and Women (SRP). The SRP served as a natural feeder to the CRFP. Personally, my career in Optical Physics owes its foundation to these programs and I will give my perspective on participation and impact of the Bell Labs SRP (1974) and CRFP (1975) programs. The Meyerhoff Scholars Program at UMBC was developed in 1988. At that time, UMBC was graduating fewer than 18 African-American STEM majors per year. In 1996 the program was opened to all students with an interest in the advancement of minorities in STEM fields. The program enjoys an overall 18-year retention rate of greater than 95% and has over 500 graduates since 1993. As of May 2006, 75% of these graduates are enrolled in graduate and/or professional programs, with 49 Ph.Ds and 20 MD/PhDs completed as of August 2006. The program challenges notions about minority achievement. Meyerhoff Scholars have changed the perceptions of those around them – the expectations of faculty who instruct them, the attitudes of students who learn beside them, and the perspectives of scientists who engage them in research.


1:03PM B3.00004 Doubling the number of physics majors who teach, MICHAEL MARDER, The University of Texas at Austin — The American Physical Society has adopted a doubling initiative to increase the number of physics majors. One of the main motivations is to increase the number of physics majors certified to teach secondary physics. I will review some of the possible strategies for reaching this goal, and discuss some of the steps we have taken with UTeach, the program for secondary science and mathematics teacher preparation at The University of Texas at Austin. I will discuss the roles of curriculum revision, financial support, and community support in convincing majors to teach. Finally, I will talk about the expansion of UTeach into engineering.
11:15 AM B4.00001 Polymer Translocation: What Can We Learn From An Exactly Solvable One-Dimensional Model?1, GARY W. SLATER, University of Ottawa — The translocation of a polymer through a narrow hole or channel is generally not a quasi-static process (as we have shown using a detailed Molecular Dynamics simulation with explicit solvent). Nevertheless, numerous analytical models have relied on this approximation/assumption in order to make progress. A simple approach is then to describe the problem in terms of the translocation coordinate (e.g., the number of monomer on the trans side of the wall), which effectively makes it a one-dimensional problem with an external driving field and a entropy-related potential landscape. Our group has exploited this simple idea to its fullest using a lattice Monte-Carlo-like model that provides exact numerical results, even for extremely rare events. In this presentation, I will explain how this simplified model is built and how it can be modified to include a variety of additional effects such as polymer stiffness or the differences between the various monomer types in a biopolymer like DNA. I will review the main results obtained to date, focusing on the transitions between the low- and high- field regimes, and between the short- and long- polymer chain limits. Finally, I will examine the role of attractive interactions between the polymer and specific sites inside the channel.

1Supported by NSERC - Canada.

11:51 AM B4.00002 DNA translocation through small channels and pores from molecular models. Hydrodynamic, electrostatic, and hybridization considerations. JUAN DE PABLO, University of Wisconsin — The flow and translocation of long DNA molecules are of considerable applied and fundamental interest. Design of effective genomic devices requires control of molecular shape and positioning at the level of microns and nanometers, and understanding the manner in which DNA is packaged into small channels and cavities is of interest to biology and medicine. This presentation will present an overview of hierarchical models and computational approaches developed by our research group to investigate the effects of confinement, hydrodynamic interactions, and salt concentration, on the structure and properties of DNA, both at equilibrium and beyond equilibrium. The talk will include a discussion of coarse grain descriptions of the flow of DNA in microfluidic and nanofluidic channels over multiple length and time scales, and a discussion of emerging, detailed models that are capable of describing melting and rehybridization at the single nucleotide level, as well as the packaging of DNA into viral capsids and small pores.

12:27PM B4.00003 Simulation studies of DNA translocation through a nanopore (†), ANIKET BHATTACHARYA, University of Central Florida — The experimental studies of voltage driven translocation of a single stranded DNA through a α-hemolysin pore, have stimulated a lot of activities as the phenomenon is rich in fundamental science involved and its prospective technical applications for detecting DNA/RNA sequences. While it is the attributes of heteropolymer translocation that are the key ingredients for prospective new sequencing methods, these experiments have generated stimulating theoretical and numerical studies directed toward a seemingly much simpler problem of homopolymer translocation through a nanopore. The earlier theoretical work of Muthukumar, Sung and Park, and by Kardar and his collaborators2 have been supplemented by more recent theoretical work by Dubbledam et. al and Panja et. al3. During this talk I will show results from Langevin dynamics simulation carried out on a coarse-grained bead-spring model of DNA-polymer both for the unbiased and driven translocation4. During the first part of the talk, after a brief review of the current theories of DNA translocation, specifically mentioning the underlying assumptions, I will compare simulation results with those predicted by different theories. Particularly, I will show numerical results for the translocation exponent α defined as \( \langle r \rangle \sim N^\alpha \) and the exponent for the s-coordinate β defined as \((s^2(r)) \sim r^\beta\), and discuss how the numerical values differ as one chooses slightly different pore width and geometry. In the second part of my talk I show how a model attractive nanopore can distinguish the sequence of a heteropolymer and discuss possibility of making a device based on this idea.

1Work done in collaboration with Kaifu Luo, Tapio Ala-Nissila, See-chen Yin, Andrey Milchev and Kurt Binder

12:03PM B4.00004 Anomalous dynamics of polymer translocation1, GERARD BARKEMA, University of Utrecht — We study the passage times of a translocating polymer of length \( N \) in three dimensions, while it passes through a narrow pore. We show that the behavior of the polymer stems from the polymer dynamics at the immediate vicinity of the pore — in particular, the memory effects in the polymer chain tension imbalance across the pore. We take as a reaction coordinate the number \( \sigma \) of the monomer residing in the pore, in the case of unbiased translocation, these memory effects cause the mobility of \( \sigma \) to be anomalous diffusion for times up to the Rouse time \( \tau_\text{R} \sim N^{3/4} \) or Zimm time \( \tau_\text{Z} \sim N^{\nu} \), without or with hydrodynamics, respectively. Here, \( \nu \) is the Flory exponent. Beyond this time, the dynamics becomes ordinary diffusion. As a consequence, the pore blockade time scales with \( \tau_\text{D} \sim N^{\nu} \) or \( \tau_\text{D} \sim N^{3/2}/N^{\nu} \) with hydrodynamics. In these cases, the pore blockade time decreases inversely with field and strength, respectively. Our theoretical framework is substantiated with high-precision computer simulations. We will show that the memory effects become more pronounced as the pore size decreases, also play a role in the dynamics of dense polymer solutions and polymer melts.

1in collaboration with D. Panja
11:51AM B5.00002 Integration of CNTs with Silicon, WILLIAM MILNE, Engineering Dept., Univ. of Cambridge — In this talk, the growth and characterization of both single and multi-walled CNTs is described and a realistic appraisal of the future of CNTs in the electronics field is provided. Although they are less likely, in the author’s opinion, to take over from silicon for use in the active devices such as transistors and diodes etc. in logic circuits their use in vias and interconnects in next generation integrated circuits is considered as being entirely feasible as is their use in transparent conducting contacts. Another major contribution to future electronics could be in conventional applications to CMOS such as their use in sensors, thermal interface materials and solder joints. A novel Liquid Crystal Over Silicon (LCOS) structure will also be discussed.

12:27PM B5.00003 Heterogeneous Integration of Materials on Si for Nanophotonics Devices, SOLOMON ASSEFA, IBM T.J. Watson Research Center — Optical interconnects are attractive candidates for achieving communication bandwidth well beyond terabit-per-second for high-performance multi-core microprocessors. Silicon has become a desirable material due to its transparency in the infrared wavelength range and the ease for integrating optical devices at the vicinity of CMOS circuitry utilizing standard processes. While state-of-the-art patterning techniques provide precise dimension control as well as pattern placement, standard doping and metallization steps enable utilization of phenomena such as carrier injection and depletion to render the devices tunable. A large progress has been made on Si-based nanophotonic devices such as modulators, switches, and wavelength division multiplexing (WDM) systems [1, 2]. To make photodetectors, however, a heterogeneous integration of other materials that absorb light in the infrared is necessary. Available in standard front-end CMOS processes for gate strain engineering, Germanium is suitable due to its high absorption coefficient at 1.3µm and 1.5µm wavelengths. Thus, Ge can be directly integrated into the process to fabricate compact photodetectors simultaneously with amplifier circuits in order to make a receiver for an optical network. Nevertheless, the integration of Ge photodetector into the CMOS process flow is very challenging due to process complexity and severe temperature constraints; as a result, photodetectors fabricated only after completing the front-end processes have been demonstrated. This talk will discuss Ge waveguide photodetectors that have been integrated into the front-end before the activation of CMOS well implants. By using the lateral seeded crystallization method wherein the Ge waveguides are melted during high-temperature dopant activation, 250-µm-long single-crystal Ge-on-insulator waveguides were fabricated. This approach eliminates the need for selective epitaxial growth of Ge, and avoids high-dose misfit dislocations formed due to lattice mismatch when growing Ge on Si substrate. The photodetectors operate at low applied bias voltages (0.5-1V) with bandwidth exceeding 40GHz.


Monday, March 16, 2009 11:00AM - 2:15PM — Session B5 FIAP: Heterogeneous Integration on Silicon 401/402

11:15AM B5.00001 Scaling Properties of High Performance Ge-Si$_x$Ge$_{1-x}$ Core-Shell Nanowire Field Effect Transistors$^1$, EMANUEL TUTUC, Microelectronics Research Center, The University of Texas at Austin — Semiconductor nanowires (NWs), namely highly anisotropic crystals with diameters of the order of a few tens of nanometers, have received increased research recently as a platform for electronics devices, motivated in part by issues associated with end of the roadmap of complementary metal-oxide-semiconductor (CMOS) device scaling. The performance advantage of such devices stems from superior electrostatic properties compared to planar devices, which in turn help increase their on-state current and on/off-state current ratio. We present recent results on the growth and fabrication of a few key NW device structures, which can potentially outperform conventional CMOS devices. By combining axial Ge NW growth, via the vapor-liquid-solid mechanism, with conformal Si$_x$Ge$_{1-x}$ growth by ultra-high-vacuum chemical vapor deposition, we demonstrate Ge-Si$_x$Ge$_{1-x}$ core-shell NW heterostructures. Transmission electron microscopy combined with energy dispersive X-ray spectroscopy show that the Si$_x$Ge$_{1-x}$ shell can be grown in-situ, epitaxial onto the Ge NW core, and that the Si/Ge shell content can be tuned depending on the growth conditions, effectively enabling band engineering in these one dimensional nanowire heterostructures. A key component in fabrication high performance nanowire field effect transistors, namely high on-state current and high on/off-state current ratio, is the fabrication of low resistance, unipolar contacts to a semiconductor nanowire. Using low energy ion implantation we demonstrate dual-gate Ge-Si$_x$Ge$_{1-x}$ core-shell nanowire field effect transistors with highly doped source and drain. We discuss the scaling properties as a function of channel length, and intrinsic carrier mobility in these devices.

$^1$Work performed in collaboration with J. N. K. Varahramyan, E.-S. Liu, S. K. Banerjee, and with support from DARPA and NSF.

1:39PM B5.00005 Integration of Ferroelectrics, Ferromagnets, and Multiferroics with Silicon, DARRELL SCHLOM, Cornell University — In this talk I will describe the epitaxial integration of ferroelectrics, ferromagnets, and materials that are both at the same time, with silicon. Until recently, "oxide" could only mean one thing to anyone working in the semiconductor industry—SiO$_2$. But oxides are an exciting class of electronic materials in their own right. Oxides exhibit the full spectrum of electronic, optical, and magnetic behavior including many functionalities not found in conventional semiconductors. Further, such oxides can be combined epitaxially not only with each other, but epitaxially with the workhorse of semiconductor technology, silicon, enabling the unparalleled variety of physical properties of oxides to be exploited in new ways for electronic applications. The specific oxides that my collaborators* and I have integrated epitaxially with silicon include EuO, ZnO, CaTiO$_3$, BaTiO$_3$, SrTiO$_3$, BaTiO$_3$, BiFeO$_3$, Pb(0.2Ti,0.8O)$_3$, and PbMg$_{1/3}$Nb$_{2/3}$O$_3$. Highlights from these systems will be presented. * The work reported was performed in collaboration with the groups of Jochen Mannhart (U. Augsburg), Chang-Beom Eom (U. Wisconsin-Madison), Ramamoorthy Ramesh (Berkeley), Jeremy Levy (U. Pittsburgh), David Muller (Cornell), Xiaoqing Pan (U. Michigan), Jürgen Schubert (Jülich), Long-Qing Chen (Penn State), Susan Trolle-McKinstry (Penn State), Yves Izdebski (Montana State), Peter Böni (TU München), Joseph Woicik (NIST), Philip Ryan (Ames), Michael Bedzyk (Northwestern), Yuni Barash (Russian Acad. Sci.), Qing Ma (Intel), and Hao Li (Motorola).
**Monday, March 16, 2009 11:15AM - 2:15PM — Session B6 FIP: Panel Discussion: Physics in Africa**

**11:15AM B6.00001 On the differences between theories of conventional and high temperature superconductors**, ALEXANDER ANIMALU, University of Nigeria — After years of successful application of the pseudo and model potential representation of electronphonon interaction to conventional (Bardeen-Cooper-Schrieffer) theory of superconductivity, we have developed a generalization (called "isosuperconductivity") that not only explains the differences between conventional and high-Tc in the cuprates and other materials but has enough predictive power to permit the current search for room temperature superconductors. We present a review of more than 30 years of effort and progress report on current research activities in this field.

**11:51AM B6.00002 Physics in Africa: The Case of South Africa**, MZAMO P. MANGALISO, National Research Foundation, South Africa & University of Massachusetts, Amherst — South Africa plays a special role in building science throughout Africa. The areas of science, particularly those related to physics, which are being developed, will be described together with the involvement of other African countries. Data will be presented that demonstrate the high attrition rate that exists especially in the science track PhD pipeline and highlight the bottleneck at the honors (fourth year) level. Programs designed to overcome this will be presented, and their success discussed. Thoughts on how to go about expanding the interactions between US scientists and South African scientists as well as with African scientists will be presented.

**12:27PM B6.00003 Physics in Africa: The Case of Senegal**, NDEYE ARAME BOYE-FAYE, University Cheikh Anta Diop, Denegal — For many years, the research activity in Senegal has been managed through the division of the Ministry of Education. In 2004 the current government established a full-fledged Ministry of Research. This has led to a renewed focus on the organization of the funding of research in Senegal. One important issue to underline is the lack of a budget line devoted to research in most of the local institutions, distinct from support for academic purposes. As a result, the research activity is funded through direct support from the government or thanks to international programs. The main tool for the government to support key research directions is the FIRST program, with a yearly budget of $700,000 US. For the last call for projects, up to 12 projects have been funded, which translates to about $58,000 US per project. The other option for research funding lies in different international programs specifically aimed at institutions within the least developed countries. The dominant ones are provided by the French-speaking community, the French-supported AIRE, the European Union framework and ICTP Abdus Salam Centre. In this general context of limited resources, physics is the least supported discipline both in terms of researchers and active laboratories. As a result, particular efforts have to be made to increase the impact of physics and the role of physicists so as to enable them to claim their proper role as the major player in making science and technology the driving forces in the development process of Africa.

**1:03PM B6.00004 Physics in Africa: The Case of Congo**, BERNARD M’PASSI-MABIALA, Marien NGouabi University — We will present a review on the state of research and education in physics in the Republic of Congo, one developing country in Central Africa. Special emphasis will be placed on the School of Science of the Marien NGouabi University located in the capital, Brazzaville. We will also discuss the impact of the Physics Department within this University as a whole. One of the main problems in Africa is the serious lack of equipment to provide adequate hands-on trainings for students and for faculty to perform forefront research. To illustrate strategies for the development of Physics in the continent, we will describe some ongoing inter-continental collaborations between our university and some neighboring countries, along with some ways for expanding the framework of the interactions between US and African physicists.

**1:39PM B6.00005 Panel Discussion**

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**11:15AM B7.00001 to be determined by you**, PATRICK DENNIS, NSF — No abstract available.

**11:51AM B7.00002 Growth laws and mechanisms of global control in bacteria**, MATTHEW SCOTT, University of Waterloo — The growth laws of Schaechter, Maaepe and Kjeldgaard are among the most striking discoveries in bacterial growth physiology: cell composition (mass/cell, RNA/cell, etc.) is a simple function of growth rate alone – irrespective of how that growth rate is established. I will review the growth laws, and discuss recent experiments that have uncovered new laws. A systems-level mathematical model is developed that suggests the growth laws arise from the partitioning of the protein synthesizing machinery of the cell (the ribosomes), and furthermore indicates a deep connection between growth rate control and central metabolism.

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**12:27PM B7.00003 Growth-rate dependent effects on bacterial gene expression**, STEFAN KLUMPP, Center for Theoretical Biological Physics, University of California at San Diego — For fast growing bacteria, which can adapt to wildly different growth conditions, changes in gene expression are often accompanied by changes in growth rates. Because the macroscopic composition of bacteria (e.g., cell size, ribosome concentration, gene copy number) is known to vary greatly for bacteria grown at different rates, significant changes in gene expression may arise 'passively' just due to the growth rate change alone. Towards a quantitative understanding of these passive effects, we analyzed quantitatively available data for the growth rate dependence of various macroscopic parameters affecting gene expression in E. coli, and predicted the growth-rate dependence of gene expression for various simple genetic circuits. For a constitutively expressed gene, the expressed protein concentration is decreased at faster growth, while weak growth-rate dependence is obtained for autorepressing genes and genes under negative control by an autorepressor. We also studied the growth-rate dependence of bistable genetic circuits and determined conditions such that bistability is found over a wide range of growth rates. Our results demonstrate that growth-rate dependent effects play an important role and must be taken into account when analyzing gene expression data under different condition. Buffering against these growth rate dependent effects may be an important requirement undermining the robust operation of endogenous genetic circuits in these bacteria, and should be a prime factor to consider in the design of robust, synthetic circuits.

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1This work was done in collaboration with Terence Hwa and Barrett Deris, and supported by Deutsche Forschungsgemeinschaft (Grants KL818/1-1 and 1-2) and the NSF through the Center for Theoretical Biological Physics (Grant PHY-0822283).
E. coli rich in resources. We apply this model to a series of past measurements, where the growth rate and rRNA-to-protein ratio have been measured for seven E. coli strains with an rRNA operon copy number ranging from one to seven (the wild-type copy number). These experiments show that growth rate markedly decreases for strains with fewer than six copies. Using the model, we were able to reproduce these measurements. We show that the model that best fits these data suggests that the volume fraction of macromolecules inside E. coli is not fixed when the rRNA operon copy number is varied. Moreover, the model predicts that increasing the copy number beyond seven results in a cytoplasm densely packed with ribosomes and proteins. Assuming that such overcrowded conditions prolonged diffusion times tend to weaken binding affinities, the model predicts that growth rate will not increase substantially beyond the wild-type growth rate, as indicated by other experiments. Our model therefore suggests that changing the rRNA operon copy number of wild-type E. coli cells growing in a constant rich environment does not substantially increase their growth rate. Other observations regarding strains with an altered rRNA operon copy number, such as nucleoid compaction and the rRNA operon feedback response, appear to be qualitatively consistent with this model. In addition, we discuss possible design principles suggested by the model and propose further experiments to test its validity.

**1:03PM B7.00004 A Coarse-Grained Biophysical Model of E. coli and Its Application to Perturbation of the rRNA Operon Copy Number**

ARBEL TADMOR, California Institute of Technology — In this work a biophysical model of Escherichia coli is presented that predicts growth rate and an effective cellular composition from an effective, coarse-grained representation of its genome. We assume that E. coli is in a state of balanced exponential steady-state growth, growing in a temporally and spatially constant environment, rich in resources. We apply this model to a series of past measurements, where the growth rate and rRNA-to-protein ratio have been measured for seven E. coli strains with an rRNA operon copy number ranging from one to seven (the wild-type copy number). These experiments show that growth rate markedly decreases for strains with fewer than six copies. Using the model, we were able to reproduce these measurements. We show that the model that best fits these data suggests that the volume fraction of macromolecules inside E. coli is not fixed when the rRNA operon copy number is varied. Moreover, the model predicts that increasing the copy number beyond seven results in a cytoplasm densely packed with ribosomes and proteins. Assuming that such overcrowded conditions prolonged diffusion times tend to weaken binding affinities, the model predicts that growth rate will not increase substantially beyond the wild-type growth rate, as indicated by other experiments. Our model therefore suggests that changing the rRNA operon copy number of wild-type E. coli cells growing in a constant rich environment does not substantially increase their growth rate. Other observations regarding strains with an altered rRNA operon copy number, such as nucleoid compaction and the rRNA operon feedback response, appear to be qualitatively consistent with this model. In addition, we discuss possible design principles suggested by the model and propose further experiments to test its validity.

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**1:39PM B7.00005 Dynamics of bacterial gene regulation**

ATUL NARANG, University of Florida — The phenomenon of diauxic growth is a classical problem of bacterial gene regulation. The most well studied example of this phenomenon is the glucose-lactose diauxie, which occurs because the expression of the lac operon is strongly repressed in the presence of glucose. This repression is often explained by appealing to molecular mechanisms such as cAMP activation and inducer exclusion. I will begin by analyzing data showing that these molecular mechanisms cannot explain the strong lac repression because they exert a relatively weak effect. I will then present a minimal model accounting only for enzyme induction and dilution, which yields strong repression despite the absence of catabolite repression and inducer exclusion. The model also explains the growth patterns observed in batch and continuous cultures of various bacterial strains and substrate mixtures. The talk will conclude with a discussion of the experimental evidence regarding positive feedback, the key component of the minimal model.

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**Monday, March 16, 2009 11:15AM - 2:15PM**

Session B8 DAMOP: Spectroscopy of Strongly Interacting Fermi Gases 414/415

**11:15AM B8.00001 Observation of Spin-Polarons in a strongly interacting Fermi liquid**

MARTIN ZWIERLEIN, Massachusetts Institute of Technology — We have observed spin-polarons in a highly imbalanced mixture of fermionic atoms using tomographic RF spectroscopy. Feshbach resonances allow to freely tune fermion interactions between the population states involved. A single spin down atom immersed in a Fermi sea of spin up atoms can do one of two things: For strong attraction, it can form a molecule with exactly one spin up partner, but for weaker interaction it will spread its attraction and surround itself with a collection of majority atoms. This spin down atom “dressed” with a spin up cloud constitutes the spin-polaron. We have observed a striking spectroscopic signature of this quasi-particle for various interaction strengths, a narrow peak in the spin down spectrum that emerges above a broad background. The narrow width signals a long lifetime of the spin-polaron, much longer than the collision rate with spin up atoms, as it must be for a proper quasi-particle. The peak position allows to directly measure the polaron energy. The broad pedestal at high energies reveals physics at short distances and is thus “molecule-like”: It is exactly matched by the spin up spectra. The comparison with the area under the polaron peak allows to directly obtain the quasi-particle weight Z. We observe a smooth transition from polarons to molecules at a critical interaction strength of 1/k_B a = 0.7. The polaron peak vanishes and spin up and spin down spectra exactly match, signalling the formation of molecules. This is the same critical interaction strength found earlier to separate a normal Fermi mixture from a superfluid molecular Bose-Einstein condensate. The spin-polarons determine the low-temperature phase diagram of imbalanced Fermi mixtures. In principle, polarons can interact with each other and should, at low enough temperatures, form a superfluid of p-wave pairs. We will present a first indication for interactions between polarons.

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**11:51AM B8.00002 Photoemission Spectroscopy for Ultracold Atoms**

DEBORAH JIN, NIST, University of Colorado — We perform momentum-resolved rf spectroscopy on a Fermi gas of potassium-40 atoms in the region of the BCS-BEC crossover. This measurement is analogous to photoemission spectroscopy, which has proven to be a powerful probe of excitation gaps in superconductors. We measure the single-particle spectral function, which is a fundamental property of a strongly interacting system and is directly predicted by many-body theories. For a strongly interacting Fermi gas near the transition temperature for the superfluid state, we find evidence for a large pairing gap.

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**12:27PM B8.00003 Competition between final-state and pairing-gap effects in the radio-frequency spectra of ultracold Fermi atoms**

GIANCARLO STRINATI, University of Camerino, Dept. of Physics — Ultracold Fermi atoms allow the realization of the crossover from Bardeen-Cooper-Schrieffer (BCS) superconductivity to Bose-Einstein condensation (BEC), by varying with continuity the attraction between fermions of different species. In this context, radio-frequency spectroscopy provides a microscopic probe to infer the nature of fermionic pairing. In the strongly-interacting regime, this pairing affects a wide temperature range comprising the critical temperature Tc, in analogy with continuity the attraction between fermions of different species. The calculation rests on the use of the BCS-RPA approximation, while in the normal phase above Tc the model includes the Azlamazov-Larkin type contribution which is familiar in the theory of “paraconductivity” fluctuations in superconductors, besides the density-of-states contribution. In both cases, the limit of a molecular spectrum is correctly recovered in the BEC regime of the crossover. A competition is revealed between pairing-gap effects which tend to push the oscillator strength toward high frequencies away from threshold and final-state effects which tend instead to pull theoscillator strength toward threshold. In addition, an energy scale associated with pairing is extracted from the spectra and related to a universal quantity recently introduced for Fermi gases.

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1Joint work of the author and Dr. Tsvi Lustig, Weizmann Institute

3Supported by NSF.
1:03PM B8.00004 Theory of RF Spectroscopy in the Normal And Superfluid Phases of Ultracold Fermi Gases, KATHRYN LEVIN, University of Chicago — In this talk we present an overview of radio frequency (RF) spectroscopy in the atomic Fermi superfluids, addressing both momentum integrated and momentum resolved experiments. A general purpose of these RF experiments is to extract the pairing gap size and we present several methodologies for accomplishing this. In addition, we discuss the effects of traps, population imbalance, and final state interactions over the entire range of temperatures. By comparing theory and experiment, we show how a broad range of experimental phenomena can be accommodated within the BCS-Leggett description of BCS-BEC crossover. We also briefly touch on commonalities between photoemission in the cuprate superconductors and RF spectroscopy in the ultracold gases.

1:39PM B8.00005 Spin polarons, Molecules and Twin Peaks in rf spectra of Fermi gases at unitarity, GEORG BRUUN, Niels Bohr Institute — We examine pairing, molecule, and spin-polaron formation in strongly-interacting Fermi gases and discuss how radio-frequency (RF) spectroscopy can reveal these phenomena. For an unpolarized gas at unitarity, we show how the double-peak structures observed in recent experiments arise due to the inhomogeneity of the trapped gas. The emergence of stable molecules in the BEC regime results in a two-peak structure in the RF spectrum with clearly visible medium effects on the low-energy part of the molecular wavefunction. For the highly-imbalanced case, we show the existence of a well-defined quasiparticle (a spin polaron) on both sides of the Feshbach resonance, we evaluate its lifetime, and we illustrate how its energy may be measured by RF spectroscopy. The main experimental features observed above the critical temperature in the recent experiments are recovered with no fitting parameters.

Monday, March 16, 2009 11:15AM - 2:15PM –
Session B9 GSNP: GSNP Student Speaker Award Session and Applications of Statistical and Nonlinear Physics in the Life Sciences 303

11:15AM B9.00001 Self-Assembly of Spherical Colloidal Particles at Low N, NATALIE ARKUS, VINOTHAN MANOHARAN, MICHAEL BRENNER, Harvard University — The number of rigid structures that a system of N particles can form grows exponentially with N. Stabilizing any one structure over all others is thus a challenging problem. We consider a system of N spherical colloidal particles that cannot deform or overlap, and which exhibit a short-range attractive force. We present a method, using graph theory and geometry, that solves for all possible rigid packings of N particles - the resultant set of packings is provably complete. We then present a mechanism that is capable of stabilizing any one structure over all others (in the zero temperature limit), and which is experimentally realizable - thereby, potentially allowing us to direct the self-assembly of a desired structure. We compare to preliminary experimental results.

11:27AM B9.00002 Liquid to solid nucleation through onion-structure droplets, KIPTON BARROS, WILLIAM KLEIN, Boston University — We start from a Landau-Ginzburg free energy and develop a theory of crystal nucleation for metastable liquids. Saddle points of the free energy represent nucleating droplets and are obtained analytically and numerically. We find nucleating droplets with hexagonal symmetry in two dimensions and bcc and icosahedral symmetries in three dimensions. Surprisingly, we also find nucleating droplets in three dimensions with a spherically symmetric structure resembling the layers of an onion. These onion-structure objects are the preferred nucleating droplets near the spinodal. We discuss recent experiments and simulations which are consistent with our predictions.

11:39AM B9.00003 Universal Scaling Relation Near Point J, THOMAS HAXTON, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania — Recently, several studies (P. Olsson and S. Teitel. Phys. Rev. Lett. 99, 178001 (2007); T. Hatano. arXiv:0803.2296; L. Berthier and T. A. Witten. arXiv:0810.4405) have indicated the existence of a dynamical phase transition at or near Point J, the point at zero temperature, zero shear stress, and a critical density where repulsive amorphous sphere packings lose rigidity. However, a universal scaling relation connecting the rheology of the jammed solid to that of the viscous liquid has been lacking. We control the temperature, strain rate, and pressure in molecular dynamics simulations to show that the steady-state rheology is described by a universal scaling relation near Point J.

11:51AM B9.00004 Exact results for currents in nonadiabatic stochastic pumps, JORDAN HORIZONITZ, University of Maryland — Biological systems abound with examples of molecular machines: assemblies of molecules that perform specific useful mechanical tasks, such as the motor proteins kinesin and myosin. Remarkably, the first steps in developing useful artificial molecular motors have been taken with the synthesis and manipulation of molecular complexes such as catenanes and rotaxanes. These developments have spurred an interest in developing theoretical frameworks which describe these mesoscopic machines that operate in the presence of thermal noise. In this talk I will analyze a generic model of molecular machines known as stochastic pumps in which useful directed motion (or current) is produced by the variation of external parameters. The main result is an exact expression for the current in the presence of nonadiabatic pumping. This expression connects to a variety of results from the field of Brownian ratchets and leads to a surprising “no-pumping” theorem: a set of conditions that guarantee no excess or pumped current. These predictions also agree with the observations on catenanes, interlocked ring molecules, made by Leigh et. al. [Nature, 424, 174 (2003)].

12:03PM B9.00005 A continuous time random walk description of the hopping dynamics in an aging polymer glass, MYA WARREN, JOERG ROTTLER, University of British Columbia — Due to the non-equilibrium nature of the glassy state, structural relaxation becomes increasingly sluggish with the wait time $t_w$ since vitrification. As a result, dynamical correlation functions age, and often obey a simple rescaling with $w = C(t, t_w) = C_0(t) + C_{age}(t/t_w)$. It has recently been shown that, to first order, scaling also applies to the distributions of local correlations and displacements (the Van Hove function). In this study, we use molecular dynamics simulations to measure the statistics of the discontinuous hopping events that characterize structural relaxations during aging. This allows us to map the particle dynamics onto a continuous time random walk, which successfully reproduces the entire distribution of displacements. Our results bear a striking resemblance to the popular trap model of aging. We find that the hop time distribution takes the form of a power law which is independent of $t_w$, whereas the time to the first hop shifts to longer times with $t_w$. This two-timescale behavior explains not only the scaling of the distribution functions for times $t \sim t_w$, but also small deviations from perfect scaling that have been observed at longer times.
1:03PM B9.00010 Estimating currents in totally asymmetric simple exclusion process with extended particles and inhomogeneous hopping rates.1, R.K.P. ZIA, Virginia Tech, JIAJIA DONG, Hamline University, B. SCHMITTMANN, Virginia Tech — Motivated by translation in protein synthesis, we study the totally asymmetric simple exclusion process with extended particles transported along a 1-D lattice with (quenched) inhomogeneous hopping rates. The particles model ribosomes, the lattice models sequences of codons, and the hopping rates reflect the aa-tRNA concentrations. Taking the latter from data for real E.Coli genes, Monte Carlo simulations allow us to find the steady state currents associated with protein production rates. An application would be to predict the effects of “silent mutations” in biological systems. In such mutations, one or more codons are replaced by others which code for the same amino-acid, so that the same protein (amino-acid chain) is synthesized by a different sequence of codons. However, the rate of production (the overall current), which depends on the details of sequence, will differ. We aim to predict the changes in these currents for all possible silent mutations. Beyond this application, this study of “quenched distribution of distributions” is expected to have far reaching implications in other areas of physics.

1Supported in part by NSF-DMR-0705152

1:15PM B9.00011 An information geometric approach to least squares minimization, MARK TRANSTRUM, BENJAMIN MACHTA, JAMES SETHNA, LASSP, Cornell University — Parameter estimation by nonlinear least squares minimization is a ubiquitous problem that has an elegant geometric interpretation: all possible parameter values induce a manifold embedded within the space of data. The minimization problem is then to find the point on the manifold closest to the origin. The standard algorithm for minimizing sums of squares, the Levenberg-Marquardt algorithm, also has geometric meaning. When the standard algorithm fails to efficiently find accurate fits to the data, geometric considerations suggest improvements. Problems involving large numbers of parameters, such as often arise in biological contexts, are notoriously difficult. We suggest an algorithm based on geodesic motion that may offer improvements over the standard algorithm for a certain class of problems.

1:27PM B9.00012 Large-Scale Organization of Glycosylation Networks, PAN-JUN KIM, University of Illinois at Urbana-Champaign, DONG-YUP LEE, National University of Singapore, HAWOONG JEONG, Korea Advanced Institute of Science and Technology — Glycosylation is a highly complex process to produce a diverse repertoire of cellular glycans that are frequently attached to proteins and lipids. Glycans participate in fundamental biological processes including molecular trafficking and clearance, cell proliferation and apoptosis, developmental biology, immune response, and pathogenesis. N-linked glycans found on proteins are formed by sequential attachments of monosaccharides with the help of a relatively small number of enzymes. Many of these enzymes can accept multiple N-linked glycans as substrates, thus generating a large number of glycan intermediates and their intermingled pathways. Motivated by the quantitative methods developed in complex network research, we investigate the large-scale organization of such N-glycosylation pathways in a mammalian cell. The uncovered results give the experimentally-testable predictions for glycosylation process, and can be applied to the engineering of therapeutic glycoproteins.
1:39PM B9.00013 Network dynamics mediated by heterogeneous topology as related to hippocampal memory management. JANE WANG, Applied Physics, UM, Ann Arbor, MI; GINA POE, Anesthesiology, UMMS, Ann Arbor, MI; MICHAEL ZOCHOWSKI, Physics, UM, Ann Arbor, MI — Hippocampal-cortical network interactions, including reactivation of recently acquired memories in the hippocampus during sleep, are key to the consolidation of memory traces to long-term storage sites in the neocortex. Network heterogeneities, in the form of regional changes in the connectivity densities of excitatory synapses, support this process in simulated hippocampal-cortical networks by regulating intrinsic network dynamics and thus mediating stimulus familiarity detection as well as selective memory consolidation. We characterize this network model by investigating dynamics due to distributed and overlapping memory structures and examine the ability of regional heterogeneities to both selectively activate in the presence of controlled stimuli and reactivate in the absence of stimuli, the former being indicative of active exploration and the latter of memory replay during sleep.

1:51PM B9.00014 The topological structure of a network formed during simulations of a reversible polymeric gel. M. WILSON, J. BILLEN, A. BALJON, SDSU, A. RABINOVITCH, Ben-Gurion U. of the Negev — We investigate the topologies of the ensemble of telechelic polymers for which we previously studied the sol/gel transition [1]. The polymers serve as “links” between “nodes,” which consist of aggregates of their associating endgroups. The number of associations and hence the topology depends on the employed temperature. Our analysis shows that the degree distribution of the systems is bimodal and consists of two Poisson distributions with different average degrees. In nodes in the distribution with the higher degree we call “superpeers,” those in the other distribution “peers.” With decreasing temperature, the fraction of superpeer nodes increases. This increase is steepest at the “jamming” transition. The eigenvalue spectra of the networks reveal that in the jammed state peers are only connected to superpeers, a topology known to be very robust. By contrast, at high temperatures peers are connected to each other as well. Due to the finite size of the polymers, our telechelic network differs from random Erdos-Renyi (ER) bimodal networks. As in many real-world networks, spatial effects play a role. After rewiring the networks obtained in the simulations, we reach the ER limit, that is, the clustering coefficients are equal to those obtained for random ER networks.

2:03PM B9.00015 Generalized fractional Fokker-Planck equation for anomalous diffusion, ALEX VEKSLER, RONY GRANEK, Ben-Gurion University of the Negev, Beer Sheva, Israel — The problem of anomalous diffusion is important for a variety of systems, such as fluids, glasses, polymers, proteins etc. It is characterized by a mean square displacement evolving in time as a power-law (z^2 = 2Dt^α). However, a Fokker-Planck-like equation which could describe a stationary Gaussian process with anomalous-diffusion behavior, such as the one described by the Generalized Langevin equation, is still missing. We propose a generalization for constant force to the fractional Fokker-Planck equation (fFP) [Metzler, R. and Klafter, J., Phys. Rep. 339 (2000), 1-77], based on a series expansion in spatial and fractional time derivatives and powers of the Fokker-Planck operator. The proposed equation, GfFP, recovers the generalized Einstein relation and leads to Gaussian distribution, in particular, for free particle diffusion. We apply GfFP to 1-D first passage time problem. The long-time asymptote of the probability distribution behaves like exp(-t^-α). This contrasts with the power-law behavior of the corresponding solutions of the fFP. We further propose to generalize GFfP for treating other outstanding problems, such as the anomalous diffusion under an harmonic potential and the Kramers’ escape problem.


11:15AM B10.00001 Switching behavior and scaling effects in ferroelectric capacitors, ALEXEI GRUVERMAN, University of Nebraska-Lincoln — In this presentation, we discuss the results of direct time-space resolved studies of domain switching behavior in micrometer capacitors by means of piezoresponse force microscopy (PFM). The PFM approach allows an insight in the mechanism of polarization reversal and its change as a function of the capacitor size and microstructure. Simultaneous visualization of the instantaneous domain configurations arising during polarization reversal and sub-ms transient current measurements allow us to establish direct relationship between the electrically measured polarization reversal signal and domain switching kinetics and determine the relative contribution of nucleation and wall motion mechanisms into polarization reversal as a function of capacitor size. Effect of microstructure on domain switching kinetics has been studied by comparing the switching behavior of polycrystalline and epitaxial capacitors. It is shown that in epitaxial capacitors the domain kinetics can be described by the classical nucleation model. In the polycrystalline capacitors, interaction of moving domain walls with microstructural defects gives rise to a completely different time dependence of polarization due to a wide distribution of local switching times. In this case the domain kinetics can be fitted by nucleation-limited switching model.

11:51AM B10.00002 Resolving Deterministic Mesoscopic Mechanisms of Local Bias-Induced Phase Transitions in Ferroelectric Materials. S.V. KALININ, S. JESSE, M.P. NIKFROV, P. MAKSYMOWYCH, N. BALKE, A. BADDORF, H.J. CHANG, A.Y. BORISEVICH, S.J. PANNYCOOK, S. CHOUDHURY, Y. LI, L.-Q. CHEN, OAK RIDGE NATIONAL LAB TEAM, PENN STATE UNIV. TEAM — Polarization switching in ferroelectric and multiferroic materials is invariably controlled by defects that act as nucleation and pinning sites. Using the synergy of high-resolution spectroscopic Piezoresponse Force Microscopy, materials systems with atomically engineered defects, and phase field modeling, we demonstrate that deterministic mesoscopic mechanisms of polarization switching can be determined. In particular, the artificial bicrystal grain boundary in (100) BiFeO_3 is found to impede ferroelectric switching, but facilitate ferroelastic switching for one of the constituent crystals. The coupling between ferroelastic domain walls and ferroelectric polarization switching is demonstrated and attributed to the kinetic effects. These studies open the pathway for probing kinetics and thermodynamics of local bias-induced phase transitions and dissipation on a single-defect level using field confinement by an SPM tip. The future potential for atomistic studies is discussed.

12:03PM B10.00003 Nanometer/Nanosecond Resolved Domain Dynamics Allowing Mapping of Distinct Nucleation and Growth Activation Energies, BRYAN HUEY, NICHOLAS POLOMOFF, VINCENT PALUMBO, JAMES BOSSE, University of Connecticut, Institute of Materials Science — A high speed variation of AFM is employed to uniquely monitor ferroelectric domain dynamics. Through pump/probe schemes, 20 nanometer resolution and 10 nanosecond temporal resolution is maintained. Consecutive images during switching therefore provide maps of nanoscale times, while domain wall growth velocities as high as 25 m/s are observed. By imaging a specific region repeatedly with several pulse amplitudes, activation energies can also be extracted as a function of position, revealing completely independent energies for nucleation and growth that are sample dependent.
12:15PM B10.00004 Optical crystallography and ferroelectric domain imaging of BaTiO$_3$ nanocrystals with tip-enhanced phonon Raman spectroscopy  
SAMUEL BERWEGER, CATALIN C. NEACSU, Department of Chemistry, University of Washington, Seattle, WA, 98195 — This study focuses on the optical characterization of BaTiO$_3$ nanocrystals, using a combination of optical crystallography and tip-enhanced phonon Raman spectroscopy. The technique allows for the detection of ferroelectric domain structures with high spatial resolution. The study demonstrates the potential of this approach for the investigation of nanocrystal materials.

12:27PM B10.00005 Effects of Surface Modification on Photo-Induced Ferroelectric Nanolithography$^1$.  
YANG SUN, CHI XU, CHIYU ZHU, ROBERT NEMANICH, Arizona State University — This study investigates the effects of surface modification on the photo-induced ferroelectric nanolithography process. The results show that surface modification can significantly affect the ferroelectric properties of the nanolithography patterns, opening new possibilities for controlling the material properties at the nanoscale.

ALEXEI GRIGORIEV, The University of Tulsa — Time-resolved studies of the polarization switching in Pb(Zr,Ti)O$_3$ capacitors reveal that the switching process is highly dependent on the applied electric field and temperature. The study provides insights into the mechanisms governing the polarization switching in these materials.


1:27PM B10.00008 Polarization rotation in epitaxially strained perovskite-oxide superlattices$.  
SERGE NAKHMANSON, Argonne National Lab — This work focuses on the polarization rotation in epitaxially strained perovskite-oxide superlattices, showing how the polarization can be rotated under certain conditions, leading to new possibilities for controlling the material properties.

1:39PM B10.00009 Local polarization discontinuities in perovskite superlattices via compensating heterointerfaces $.  
EAMONN MURRAY, DAVID VANDERBILT, Rutgers University — This study demonstrates how local polarization discontinuities can be compensated using heterointerfaces, leading to materials with enhanced ferroelectric properties.

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$^1$Supported in part by NSF, DOE, and Research Corporation.

$^2$Supported in part by NSF grant DMR -0805353.

$^3$Work supported under contract No. DE-AC02-06CH11357 between UChicago Argonne, LLC and the Department of Energy.

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1:51PM B10.00010 Enhanced piezoelectricity in PbTiO$_3$/BaTiO$_3$ superlattices, VALENTINO R. COOPER, Oak Ridge National Laboratory, KARIN M. RABE, Rutgers University — Short period ferroelectric/ferroelectric PbTiO$_3$ (PTO)/BaTiO$_3$ (BTO) superlattices are studied using density functional theory. Contrary to the trends in paraelectric/ferroelectric superlattices the polarization remains nearly constant for PTO concentrations below 50%. In addition, a significant decrease in the c/a ratio below the PTO values is observed. We predict an enhancement in the $d_{33}$ piezoelectric coefficient peaking at ~75% PTO concentration due to the different polarization-strain coupling in PTO and BTO layers. Further analysis with a superlattice effective Hamiltonian reveals that these trends are bulk properties which are a consequence of the reduced $P$ brought about by the polarization saturation in the BTO layers.

2:03PM B10.00011 ABSTRACT WITHDRAWN —

Monday, March 16, 2009 11:15AM - 2:03PM —
Session B11 DMP: Focus Session: Transport Properties of Nanostructures I: Surface Assemblies and Films 305

11:15AM B11.00001 Following elemental chemical steps by imaging molecular orbitals by STM, PETER LILJEROTH, University of Utrecht — Probing the electronic structure of molecules by STM is complicated by the strong interaction of the molecular orbitals with the metal substrate.[1,2] Adiabatically increasing the ultrathin insulating film alleviates this problem and allows direct imaging of molecular orbitals in real space.[1] This approach will be illustrated by two examples: characterizing the operation of a single-molecule switch and controlling and monitoring the formation of an organometallic complex. The inner hydrogens in the central cavity of a naphthalocyanine molecule can be switched between two equivalent positions.[3] This process (hydrogen tautomerization reaction) can be initiated in a controlled fashion by excitation induced by the inelastic tunnelling current. The tautomerization reaction can be followed by resonant tunnelling through the LUMO of the molecule and is expressed as considerable changes in the conductivity. In addition, we demonstrate a coupling of the switching process so that the charge injection in one molecule induces tautomerization in an adjacent molecule. The other example will consider constructing an organometallic complex from individual organic molecules and metal atoms by STM manipulation on the ultrathin insulating film. The manipulation process and the associated changes in the molecular orbitals (energy, spatial extension, symmetry) can be followed STM imaging and spectroscopy.


1Work in collaboration with Jascha Repp and Gerhard Meyer.

11:51AM B11.00002 Apparent anomaly in electron scattering in Ag nanostructures*, ELLEN D. WILLIAMS, CHENGANG TAO, WILLIAM C. CULLEN, Dept. of Physics, U. of Maryland - College Park — Electron scattering from diffusing atoms can be visualized via the effects of the corresponding force that biases atomic motion, the “electromigration force”. Using a combination of scanning tunneling microscopy and scanning electron microscopy, we investigate electron scattering via the biased motion of monatomic islands and CuO-decorated steps on Ag(111) surfaces in the presence of large current density ($j_{bulk} = 6.7\times10^{9}$ A/m$^2$). For monatomic adatom islands, the biased motion is opposite to the current direction and thus parallel to the direction of momentum transfer (the “wind force” direction), while vacancy islands move oppositely. The measured drift velocity $v$ as a function of the island radius $R$, $vR = 1.9$nm$^2$/s, yields an anomalously large effective force per boundary atom $-0.06$ meV/nm . An effective scattering force of similar magnitude is also observed via current-induced curvature of CuO-decorated line-boundaries. Possible mechanisms for this effect, including current crowding, charge transfer and local heating, will be discussed. 1. A. Bondarchuk, et al. Phys. Rev. Lett. 99, 206801 (2007)

1Supported by the UMD-NSF-MRSEC grant # DMR 0520471.

12:03PM B11.00003 Orbital-resolved polaron states in CdSe dots and rods probed by scanning tunnelling spectroscopy, PETER LILJEROTH, ZHIXIANG SUN, INGMAR SWART, University of Utrecht, CHRISTOPHE DELERUE, IEMN-Dept. ISEN, DANIEL VANMAEKELBERGH, University of Utrecht — Despite the extensive knowledge of phonons in semiconductor crystals, the polaron states formed by the coupling between phonons and single electronic orbitals have not been measured directly due to the negligible spacing between the energy levels in conventional semiconductors. This can be overcome in semiconductor nanocrystals that have discrete energy levels due to quantum confinement. Here, we present scanning tunneling spectroscopy results on CdSe dots and rods showing the single- electron polaron energy levels with their phonon replica. We measure the spacing and intensity of the replica, and derive the electron-phonon coupling strength for different orbital symmetries. The effect of multiple added electrons on the coupling strength can be assessed under shell-filling conditions. Our results show the formation of polaron eigenstates arising from Fröhlich coupling of an electron to longitudinal phonons with a coupling strength that depends considerably on the size and shape of the nanocrystals. The results are important for understanding electron transport in zero and one-dimensional semiconductors and the intra-band relaxation of hot carriers in quantum dots.

12:15PM B11.00004 Morphology and transport properties of self-assembled, ligand-exchanged PbSe nanocrystal arrays, CHING-TZU CHEN, IBM Thomas J Watson Research Center, WEON-KYU KOH, CHRISTOPHER MURRAY, Department of Chemistry, University of Pennsylvania, CHANG C. TSUEI, IBM Thomas J Watson Research Center — Self-assembled PbSe nanocrystal (NC) arrays have shown strong potential as a viable candidate for producing large-scale quantum dot superlattices. Such superlattices not only have significant technological implications, but they also serve as a model system for simulating strongly correlated transition-metal oxides. At present, highly-ordered PbSe NC arrays can be reproducibly prepared on structured Si-substrates by drop-casting PbSe solution in controlled environments. The as-grown superlattice films are nearly insulating, and post-processing ligand exchange is necessary to induce conduction. However, the lack of understanding of the ligand exchange processes has been a bottleneck to reliably producing highly-ordered conductive arrays. In this talk, we report on in-depth characterizations of the PbSe NC films treated with various ligand molecules in different solvents. The effect of a range of ligands and solvents on the film morphology will be discussed in details. Preliminary temperature-dependent transport and noise studies will be presented.
12:27PM B11.00005 Tunneling Spectroscopy of Ultrathin Insulating Films: Cu$_2$N on Cu(100)\textsuperscript{1}

CHARLES RUGGIERO, TAEYOUNG CHOI, JAY GUPTA, The Ohio State University — Insulating films of only a few atomic layers offer insight into the evolution of electronic structure at the nanoscale. We report scanning tunneling microscopy (STM) studies of monolayer Cu$_2$N films grown on Cu(100). Our tunneling spectra indicate that Cu$_2$N acts as an insulator, with a band gap that exceeds 4 eV \textsuperscript{1}. We study changes in this electronic structure with size, ranging from few-atom islands to complete films. We find that the conduction band edge first emerges in few-atom islands, and shifts toward lower energy with increasing island size. Images of the local density of states show standing wave patterns consistent with the confinement of electrons to these 2D islands.

Measurements of the tunneling barrier height and image potential states indicate that the Cu$_2$N work function is ~0.9 eV larger than bare Cu. This suggests a significant surface dipole, consistent with charge transfer predicted by theory. http://www.physics.ohio-state.edu/~jgupta

\textsuperscript{1} NSF CAREER (DMR-0645451).

12:39PM B11.00006 Ambipolar Ballistic Electron Emission Microscopy (BEEM) Studies of Gate-field Modified Schottky Barriers(SBs). Y.L. CHE, J.P. PELZ, The Ohio State University — Gate-field modified SBs are important for “Schottky Barrier FETs” \textsuperscript{1}, and could be used to control spin and charge injection into other semiconductor device structures. We have made the first \textit{ambipolar} BEEM measurements on Au/Si SBs that can be changed from effective n-type to p-type by applying a positive or negative back-gate bias, respectively. Samples were fabricated using SIMOX silicon-on-insulator wafers (35nm Si/150nm SiO$_2$/p-Si substrate), with Ti/Au and Pt pads as ohmic contacts for n-type and p-type operation, respectively. The local SB heights at 80K for electrons and holes were measured at the \textit{same location} to be ~0.785eV and ~0.332eV respectively, which correspond to intrinsic SBHs of ~0.84eV and ~0.36eV after accounting for image force lowering. These sum to 1.20eV, close to the ~1.17eV Si bandgap at 80K. We will discuss on-going measurements of the dependence of the local SBH on temperature, back-gate bias, Si film thickness, and bias between the Schottky and ohmic contacts. Future work will investigate local variations of the conduction and valence bands due to local “geometry-induced” electric fields in nanostructured contacts. Work supported by National Science Foundation Grants No. DMR-0505165 and DMR-0909237 \textsuperscript{1}


12:51PM B11.00007 Temperature dependence of lateral hot-electron spreading in Au films using Cross-Sectional Ballistic Electron Emission Microscopy. C. MARGINEAN, J.P. PELZ, The Ohio State University — Cross-sectional ballistic electron emission microscopy (XBEEM) was used to investigate the temperature dependence of hot-electron lateral spreading in metal films. A sequence of GaAs QWs of 1 to 15 nm width (separated by 200nm Al$_{0.3}$Ga$_{0.7}$As barrier layers) were cleaved \textit{ex situ}, and then 10 nm-thick of Au was thermally deposited on the cleaved edge to form Au Schottky barrier (SB) “nanoaperture” contacts \textsuperscript{1}. Previous XBEEM results showed an unexpectedly large hot-electron lateral spreading at room temperature consistent with multiple electron scattering inside the metal film \textsuperscript{2}. If phonon scattering of hot-electrons is significant in Au films (as previously suggested \textsuperscript{3}), then the lateral spreading should increase at lower temperature. However, we found that the lateral spreading at 80K was almost the same as at room temperature, suggesting that electron-phonon scattering is not the dominant scattering mechanism. We will also discuss the temperature dependence of the BEEM current amplitude, as well as Monte-Carlo simulations of the lateral spreading process. Work supported by NSF Grant No. DMR-0505165. \textsuperscript{1} C. Tivarus, \textit{et al}. PRL 94, 206803 (2005) \textsuperscript{2} C. Tivarus et al., APL 87, 182105 (2005) \textsuperscript{3} L. D. Bell, PRL 77, 319007 (1996).

1:03PM B11.00008 Classical size effect in nanometric Cu films: the dominant role of grain boundary scattering. D. CHOI, Dept. of Mater. Sci. and Eng., Carnegie Mellon Univ., Pittsburgh, PA 15213, T. SUN, A. WARREN, B. YAO, AMPAC, Univ. of Central Florida, Orlando FL 32816, A. DARBAL, K. BARMAK, Dept. of Mater. Sci. and Eng., Carnegie Mellon Univ., Pittsburgh, PA 15213, M. TONEY, Standard Synchrotron Radiation Laboratory, Menlo Park, CA 94025, R. PEALE, Dept. of Physics, Univ. of Central Florida, Orlando FL 32816, K. COFFEY, AMPAC, Univ. of Central Florida, Orlando FL 32816 — Surface and grain boundary electron scattering contribute significantly to resistivity as the dimensions of polycrystalline metallic conductors are reduced to, and below, the electron mean free path. In this work, a methodology is reported to independently evaluate surface and grain boundary scattering in encapsulated polycrystalline Cu thin films, with thicknesses of 28-158 nm, grain sizes of 35-466 nm, and interface roughnesses of 0.2-2 nm. The film resistivity, measured at both room temperature and at 4.2 K, is compared for samples having different grain sizes and film thicknesses. The resistivity contribution from grain boundary scattering is found to be dominant in SiO$_2$/Cu/SiO$_2$ and Ta/ SiO$_2$/Cu/Ta/SiO$_2$ films. Resistivity data for a third set of samples, namely SiO$_2$/TaSiN$_x$/Cu/TaSiN$_x$/SiO$_2$, will also be presented.

1:15PM B11.00009 Crystal Orientation Imaging of Nanometric Metal Films in the Transmission Electron Microscope. A. DARBAL, K. BARMAK, N. T. NUHFER, Dept. of Mater. Sci. and Eng., Carnegie Mellon Univ., Pittsburgh, PA 15213, D. J. DINGLEY, G. MEADEN, EBSSD Consultants, Salt Lake City, UT 84105, J. MICHAEL, Sandia National Laboratories, Albuquerque, NM 87185, T. SUN, B. YAO, K. R. COFFEY, AMPAC, Univ. of Central Florida, Orlando FL 32816 — A reliable method for orientation mapping of nanocrystals is crucial to the study of the impact of grain boundaries on resistivity increase of metal films as thickness is reduced (classical size effect). Here we report on the use of the Automated Crystallography (ACT) system for high-resolution grain and orientation mapping in the TEM. The samples for the study were a 50 nm-thick Pt film annealed at 800 °C and a 40 nm-thick Cu film annealed at 450 °C. In ACT, the diffraction pattern for a given point is constructed by analyzing its intensity variation in a series of dark field images obtained using hollow-cone illumination. The reconstructed diffraction pattern for every point is indexed to obtain the orientation map. The sensitivity of the orientation imaging results to details of sample preparation, data acquisition and choice of indexing parameters is discussed.

1:27PM B11.00010 Controlling the assembly and electronic properties of solution processed CNT devices: From large area arrays to individual CNT\textsuperscript{1}. SAIFUL I. KHONDAKER, PAUL STOKES, YODCHAY JOMPOL, SHASHANK SHEKHAR, Nanoscience Technology Center and Department of Physics University of Central Florida, Orlando, FL 32826 — Single walled carbon nanotubes (SWNTs) are considered to be ideal components for nanoelectronic devices because of their exception electronic properties. Integration of these nanostructures into electronic circuits requires the precise positioning of them in different architectures. Here we will summarize our recent progress on the directed assembly of SWNTs using AC dielectrophoresis (DEP). SWNTs are assembled from a surfactant free commercially available aqueous solution using a non uniform electric field. By controlling the electric field strength, frequency, density of solution and novel fabrication techniques, we are able to control the assembly of SWNT from dense arrays mimicking electric flux to single SWNT devices with high yield. Electronic transport properties of field effect transistors and single electron transistors fabricated from such assembly will be discussed.

\textsuperscript{1} This work is partially supported by NSF-CARRER award ECS-0748091.
films. That the PV response of suspended films in vacuum is mainly driven by thermal mechanisms. Finally, we were able to reverse the sign of the PV by changing the doping state of the carbon nanotube films. Thus, monitoring the magnitude of the PV appears as a powerful tool for evaluating the doping state of suspended films.

1:51PM B11.00012 Carrier Type and Transport Characteristics of a-B3C. MARCUS SKY DRIVER, SAAD JANJUA, SUDARSHAN KARKI, DAESUHEUM YEOUN, ANTHONY CARUSO, Dept. of Physics, University of Missouri - Kansas City, CARUSO RESEARCH GROUP TEAM — Boron carbide has many technological applications, including radiation hard semiconducting applications; the most popular of which is volatlic transduction. Structural defects are known to exist, whose implications in defining the majority carrier type is important, yet unclear. Gaining greater insight into the local physical structure and transport character is crucial toward optimizing the volatile behavior. Subsequently, gaining information about the majority carrier and carrier concentration from Hall effect and band structure from photoemission spectroscopy gives insight into the electronic structure and transport of boron-rich carbides. Boron carbides are predominately p-type due to their electron deficiency, but it has been suggested that the electron as a majority carrier may also exist. Preliminary studies including Hall effect, photoemission and extended X-ray absorption fine structure will be discussed within the context of amorphous boron carbides with respect to the carrier properties and physical structure for various growth conditions, within the context of local structural defects.


11:15AM B12.00001 Effects of shadowing and steering in oblique incidence epitaxial growth1. YUNUSIC SHIM, Department of Physics and Astronomy, University of Toledo — Recently the fabrication of novel nanostructures by oblique deposition has drawn much attention due to their potential application in electronic and mechanical devices as well as the interesting morphologies observed in various experiments, such as nanorods, nanocolums, and nanohelicoids. Unlike self-organization by misfit strain in heteroepitaxial growth, oblique deposition provides a relatively direct way of controlling surface structures of growing films. Recent experiments indicate that oblique incidence deposition can significantly alter materials properties such as surface roughness, magnetic anisotropy, optical transmittance, and porosity. After a review of these experimental results, we first show that a series of morphological transitions observed in oblique incidence Cu/Cu(100) growth near room temperature can be explained primarily by geometrical shadowing effects [1]. We then discuss the modifying effects of steering due to short-range and long-range attraction [2] as well as of substrate rotation on the surface morphology. Finally, we present the results of recent multiscale simulations of Cu/Cu(100) growth at lower temperature (T = 160 - 200 K) [3] as well as of parallel accelerated dynamics and molecular dynamics simulations at very low temperature [4]. Based on these simulations we have been able to explain a number of recent intriguing but previously unexplained experimental results including the strong dependence of the surface morphology and roughening behavior on temperature as well as the development of compressive strain in metal thin film growth.


1Supported by NSF grant DMR-0606307.

11:51AM B12.00002 Diffusion of two-dimensional Cu islets on Ag(111) studied with the Molecular Dynamics Method. SADAR S. HAYAT, The Islamia University of Bahawalpur, MARISOL ALCANTARA ORTIGOZA, TALAT S. RAHMAN, University of Central Florida — Our molecular dynamics simulations (at 300, 500 and 700 K) of the diffusion of two-dimensional Cu$_n$ islets (1≤n≤9) on Ag(111) using many-body potentials yield an Arrenius behavior. Concentrated motion is seen to dominate the diffusion of smaller islets (2-4 atoms) whereas multiple-atom, shape-adjusting processes control the diffusion of the larger ones. Although the effective energy barrier scales with islet size, the barriers do not change considerably for islands containing 4 to 9 atoms (they are ~220 ± 37 meV). While the diffusion barrier for Cu monomers on Ag(111) is higher than that on Cu(111) (both in experiment and theory), the situation reverses starting from the dimer. Our results for monomer and dimer are in excellent agreement with those extracted from experiments. On comparing our results with those for Cu islets on Cu(111), we find that the comparatively large Ag-Ag bond-length sets the contrast between Cu monomer diffusion on Cu(111) and on Ag(111). The diffusivity of Cu dimer, however, is boosted on Ag(111) by the competition between optimizing the Cu-Cu and the Cu-Ag bonds. For larger islets (3-9 atoms) our results reveal several novel diffusion processes, including those in which an islet-atom climbs atop. Morgenstern et al. PRL93, 056102 (2005). Work supported by NSF-ITR 0428826.

12:03PM B12.00003 Atomic structure determination of the (001) surface of the semimetal Bi by STM and LEED J. SUN, J. WANG, Dept. of Physics, Univ. of New Hampshire; J. WELLS, NTNU, Trondheim, Norway; PH. HOFMANN, Institute for Storage Ring Facilities, University of Aarhus, Denmark; K. POHL, Dept. of Physics, Univ. of New Hampshire — The Bi surfaces differ from the semimetal bulk due to the metallic surface states, induced by the symmetry breaking and strong spin-orbit interaction. All Bi surface states studied are spatially confined to the first layer. Bi(001) is a notable exception with deeply penetrating states, which could have a significant effect on the bulk properties of nanostructures. This work presents surface morphology observation by STM and atomic structure determination by LEED, which are expected to be closely related to the electronic properties. STM shows an unconstructed surface and wide terraces with double-layer step heights of about 3.76 ± 0.02 Å. We also identify the short termination by obtaining unstable single step heights via special sputtering operations. In the LEED analysis, the termination with an intact bilayer also results in a much better agreement between calculated and measured intensities than the broken bilayer. Strong multilayer oscillatory relaxations (about 10%) are found to reach deep into the fifth layer, which can be seen as the structural response to the unusually deep surface state penetration at this surface. The measured relaxations agree well with those from first-principles calculations.
12:15PM B12.00004 Thermal-stability of Pd-Cu surface alloys investigated at the nanometer-scale by LEEM-IV analysis . E. BUSSMANN, Sandia National Labs, NM — Pd-Cu(100) surface alloys are interesting as model systems for metal/metal epitaxy, as well as for their catalytic properties, and as coatings, e.g. for electromigration resistance. We employ the LEEM-IV technique, with 8.5 nm spatial resolution and submonolayer chemical sensitivity, to investigate Pd interdiffusion into the Cu(100) surface. The LEEM-IV technique is sensitive to the layer-by-layer composition down to the fourth subsurface layer. After annealing a 0.4 ML Pd surface alloy at around 540 K, some regions of the surface develop a Cu$_3$Pd structure, a familiar bulk alloy phase. In other regions, the surface Pd concentration becomes dilute due to Pd diffusion into the bulk. We estimate the thermal activation barrier to Pd diffusion from the surface alloy into Cu bulk to be 1.7±0.15 eV. The LEEM allows real-time, real-space, observation of the interdiffusion process, and the concurrent evolution of the surface structure, at the nanometer scale. Sandia is operated by Sandia Corp., a Lockheed Martin Company, for the U. S. DOE’s NNSA under Contract No. DE-AC04-94AL85000. Work at UNH is funded by the NSF under Grant No. DMR-0134933.

12:27PM B12.00005 Bistability of Nanoscale Ag Islands on Anisotropic Si(111)-(4x1)-In Surface Stress Template . MIAO LIU, University of Utah, YAOYI LI, Tsinghua University, DECAI YU, University of Utah, JINFENG JIA, QIKUN XUE, Tsinghua University, FENG LIU, University of Utah, DAYAN MA, Xi’an Jiaotong University, XUCUN MA, Chinese Academy of Sciences — We present a combined experimental and theoretical study of stability of Ag nanofilms grown on Si(111)-(4x1)-In surface. Experiments show the existence of two stability regimes: a conventional regime at low temperature where only one island shape is stable, and an unconventional regime at room temperature (RT) where isotropic compact islands coexist with anisotropic elongated ones. First-principles calculations show the unusual bistability at RT arises from the fact that the Ag nanofilms are under anisotropic stress, further supported by a continuum model of island shape evolution as a function of island size.

12:39PM B12.00006 Impurities in Vacuum Deposition: Effect on Island Nucleation and Surface Morphologies1, 2. ALBERTO PIMPINELLI, Univ. of Maryland, College Park (UM) & U.B.P.Clermont-2 & Science Attaque, French Consulate, Houston, AJMI BH.HAMOUDA, UM & Univ. Monastir, Tunisia, T. L. EINSTEIN, UM — The effect of impurities on epitaxial growth in the monolayer regime is studied using kinetic Monte Carlo simulations of two species solid-on-solid growth model. Both species are mobile, and attractive interactions among adatoms and between adatoms and impurities are incorporated. Impurities can be codeposited with the growing material or predeposited prior to growth. We discuss the peculiar morphologies observed in copper on copper deposition on vicinal surfaces, and argue that only the presence of impurities can explain all observed features3. We also investigate the effect on island morphology using a recently developed approach based on capture zone distributions.

1Work at UM supported by the MRSEC, NSF Grant DMR 05-20471

12:51PM B12.00007 Interface evolution and cluster formation during de-wetting of thin solid films . ADI CONSTANTINESCU, LEONARDO GOLUBOVIC, West Virginia University, ARTEM LEVANDOVSKY, University of California Riverside — Morphology evolution of solid thin films is investigated within a continuum interface dynamics model that incorporates both the interface relaxation and the long range de-wetting interactions. The model is used to explore the cluster formation phenomena seen on the surfaces of polymeric and metallic thin films. Via numerical simulations and analytic arguments, we obtain the scaling laws governing the coarsening growth of these clusters. These scaling laws are found to be super-universal at long time scales: They do not depend on the dimensionality of the film substrate and the nature of the long range de-wetting interactions, as documented by our numerical simulations on 1-d and 2-d substrates with de-wetting interactions of various forms. However, for the physically interesting 2-d substrates, the long range interactions introduce a distinct early time scaling behavior that persists over many decades of time and may be significant for the understanding of the current experimental phenomenology.

1:03PM B12.00008 First-passage time approach to kinetic Monte Carlo simulations of metal(100) growth1, 2. GIRIDHAR NANDIPATI, YUNUSIC SHIM, JACQUES AMAR, University of Toledo — One of the difficulties in carrying out realistic kinetic Monte Carlo simulations is the existence of rapid, repetitive low-barrier processes which can dramatically slow down the simulation. For example, in metal(100) growth the rate for edge-diffusion can be very fast even at moderate temperatures, while the barriers for edge-detachment and corner rounding are relatively high. While one approach to this problem is to artificially reduce the rate of edge-diffusion, such an approach can significantly alter the thin-film evolution. To address this problem while still preserving the relative rates for all processes, we have developed a modified KMC method in which edge-diffusion and corner-rounding are treated using a first-passage time formalism, while the remaining processes are treated as in normal KMC. In simulations of an effective-medium theory (EMT) based model of Cu/Cu(100) growth at T = 200 K and above we find that a speed-up of several orders of magnitude is possible, without sacrificing accuracy. Preliminary results for Cu/Cu(100) growth at high temperatures will also be presented.

1Supported by NSF DMR-0606307

1:15PM B12.00009 Growth morphology of ultra-thin Ni films on Pd (100)1, 2. PATRICIO HÄBERLE, CAROLINA PARRA, UTFSM, Valparaiso — A series of thin Ni films with thicknesses between 0.2 ML to 13 ML were deposited on a Pd(100) substrate at room temperature (RT). Growth morphology was investigated using scanning tunneling microscopy (STM). The STM images indicate the existence of three different growth modes. Up to 6.5 ML, Ni films grow pseudomorphically, consistent with a face-centered tetragonal (fct) structure. From 6.5 ML to 10.5 ML a new interlayer distance of 1.0 ± 0.1 Å is established. The new structure is accompanied by the appearance of an arrangement of filaments on the top layer. These filaments are presumably related to a strain relief mechanism of the fct films. Finally above 10.5 ML the Ni films recover their face-centered cubic (fcc) lattice constants. The filaments evolve to form a net-like structure over the whole surface. Preliminary data indicates the magnetic properties of the layers are linked to the evolution of the film’s structure.

1Acknowledgements to grant ACT 027, PBCT, Chile

1:27PM B12.00010 Dynamical LEED analysis of a quasicrystalline Cu film using periodic approximant structure models . RENEE DIEHL, Penn State University, KATARIINA PUSSI, Lappeenranta University of Technology — Quasicrystalline surfaces pose a challenge to diffraction techniques since they have no periodicity. They do, however, have good long-range order and produce diffraction patterns with sharp peaks. Copper grows on the 5-fold surface of i-Al-Pd-Mn in a layer-by-layer mode. Although its atomic structure cannot be determined by STM, the diffraction pattern from a 5-layer thick film consists of sharp peaks and streaks, the location of which indicate that this film consists of an aperiodic array of rows of periodically-spaced Cu atoms. We have applied the method of periodic approximants in a dynamical LEED analysis of the structure of this quasiperiodic copper film to determine the atomic structure of the Cu film. This analysis indicates that the Cu film has a distorted cubic structure that conforms to the quasiperiodic substrate structure, providing an example of periodic-aperiodic structure matching. This research is supported by NSF-DMR-0505160 and the Academy of Finland.
1:39PM B12.00011 Theoretical Study of Adsorbates-induced Restructuring of Pb flat-top mesa in the Quantum Regime\(^1\), WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, ALEXANDER KHAIJ-TOORIANS, University of Texas at Austin & University of Hamburg, CHIH-KANG SHIH, University of Texas at Austin, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee — Based on first-principles total energy calculations, we study the adsorption and diffusion of a series of metal adsorbates (Fe, Co and Cs) on flat-top Pb mesas, focusing on their influence on the morphology of the mesas. We found that single Fe and Co atoms can easily dive into the substrate interstitial sites by overcoming a small energy barrier upon deposition onto the mesa top. In contrast, Cs atoms are able to substitute first-layer Pb atoms via a phase exchange process resulting in a surface alloy. This induces a dramatic change on the surface morphology of these mesas as observed in recent experiments. The modification of the transformation is characterized by the emergence of Cs-decorated monolayer-high Pb islands which are predominantly formed on quantum mechanically unstable regions of the Pb mesas. Connections with experimental observations in other related systems will also be discussed.

\(^{1}\)Supported by DMSE/BES of USDOE and USNSF.

1:51PM B12.00012 Stress development and relaxation during early stages of oxidation of metals and alloys\(^1\), GUANGWEN ZHOU, CHANGHONG KE, State University of New York, Binghamton, JUDITH YANG, University of Pittsburgh, JEFFREY EASTMAN, JOHN PEARSON, Argonne National Laboratory — It has been long recognized that oxidation of metals results in the generation of stresses and these stresses play an important role in shaping the microstructure of oxide films. However, the mechanism governing the stress development and relaxation during early stages of oxidation of metals and alloys is still to a significant degree unclear. Using a combination of in-situ ultra-high vacuum (UHV) transmission electron microscopy (TEM) and finite element method, we show how oxidation-induced stresses can be used to tailor the initial oxide formation during early-stage oxidation of Cu(100) and Cu-Au(100). From analysis of the observed morphological evolution of Cu\(_2\)O nanoslands, we establish a close relationship between the stresses generated from the oxide growth and the thermodynamic selection of nanoscale morphology of the oxide film. We expect that our results have implications for controlled production of novel oxide nanostructures through controlling the oxidation-induced stresses via oxidation temperature or alloying.

\(^{1}\)This work was supported by the National Science Foundation (NSF) under the grant No. 0825737

2:03PM B12.00013 Studies of oxidation of the Cu(100) surface using low energy positrons. , W.B. MADDox, N.G. FAZLEEw, A.H. WEISS, Department of Physics, University of Texas at Arlington — Changes in the surface of an oxidized Cu(100) single crystal resulting from vacuum annealing have been investigated using positron annihilation induced Auger electron spectroscopy (PAES). PAES measurements show a large increase in the intensity of the positron annihilation induced Cu M\(_{2,3}\)VV Auger peak as the sample is subjected to a series of Isochroinal anneals in vacuum up to annealing temperature 300° C. The intensity then decreases monotonically as the annealing temperature is increased to ~600° C. Experimental PAES results are analyzed by performing calculations of positron surface states and annihilation probabilities of surface-trapped positrons with relevant core electrons taking into account the charge redistribution at the surface, surface reconstructions, and electron-positron correlations effects. Possible explanation for the observed behavior of the intensity of positron annihilation induced Cu M\(_{2,3}\)VV Auger peak with changes of the annealing temperature is proposed.

Monday, March 16, 2009 11:15AM - 1:51PM — Session B13 SPS Undergraduate Research I 309

11:15AM B13.00001 Introductory Physics Experiments Using the Wiimote , WILLIAM SOMERS, FRANK ROONEY, ROMULO CHOCA, The College of New Jersey — The WII, a video game console, is a very popular device with millions of units sold worldwide over the past two years. Although computationally it is not a powerful machine, to a physics educator its most important components can be its controllers. The Wiimote (or remote) controller contains three accelerometers, an infrared detector, and Bluetooth connectivity at a relatively low price. Thanks to available open source code, any PC with Bluetooth capability can detect the information sent out by the Wiimote. We have designed several experiments for introductory physics courses that make use of the accelerometers and Bluetooth connectivity. We have adapted the Wiimote to measure the variable acceleration in simple motion, centripetal and tangential accelerations in circular motion, and the accelerations generated when students lift weights. We present the results of our experiments and compare them with those obtained when using motion and/or force sensors.

11:27AM B13.00002 Binary Orbital Motion of Electrically Charged Spheres in Weightlessness.\(^1\), LULU LI, BRAD ATKINS, GAVIN FRANKS, JOSHUA FUCHS, CHASE SLIGER, JENNIFER THOMPSON, RHODES BINARY ORBIT TEAM — The similar mathematical forms of Coulombs Law of Electrostatics and Newton’s Law of Gravitation predict that two oppositely charged spheres should be able to move in a binary orbit about their center of mass using only the electric force as the force of attraction. To test this prediction, we conducted an experiment in July 2008 aboard a specialized C-9B aircraft in NASA’s Microgravity University Program which simulates the conditions of weightlessness. We successfully achieved multiple binary orbits between the two spheres. The orbital motion was analyzed using VideoPoint software to measure the orbital interaction of the spheres.

\(^{1}\)NASA; 07-08 SPS undergraduate research grant

11:39AM B13.00003 Dynamics of a charged Kapitza’s pendulum interacting with radiation in thermal equilibrium , JORGE HERNANDEZ GOMEZ, PAULINA PRADLE SOTO, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico — The considered system is a Kapitza’s pendulum that consists of a disk that spins at constant angular velocity, from which edge is attached a massless rigid rod with an electrically charged bob. The system is studied theoretically and experimentally. The motion equations are settled and solved both, analytically under the small oscillation assumption considering the interaction of the system with black body radiation as a perturbation, and in the general case using numerical algorithms. The pendulum’s dynamics is studied varying both initial conditions and parameters in small steps. In order to identify regions of stable and chaotic motion, Lyapunov’s exponents are calculated. Phase and configuration spaces are plotted to notice periodic and erratic behaviors. Poincare sections and fast Fourier transforms are obtained to identify resonance cases.

11:51AM B13.00004 Electrical energy dissipation in superconducting niobium rings\(^1\), E. M. DOWDELL, K. M. CHIOLA, E. T. ROSAURI, J. D. HETTINGER, Department of Physics and Astronomy, Rowan University — Niobium rings were made from films synthesized using sputtering process. Rings and wires were defined in the films using standard photolithographic techniques followed by wet etching. Three rings were fabricated with different diameters and wire widths. One microbridge was created for direct electrical transport measurements. V-I characteristics of the superconducting niobium microbridge were measured at temperatures below 7K and at magnetic fields up to 2T. Dissipation was induced in the superconducting niobium rings by ramping the magnetic field and measuring Faraday’s Law. The current induced was measured through the magnetic moment and the simple expression \(\mu_{edip}=IA\). We will correlate the magnetically induced measurements with those made directly on the microbridge to investigate this method as a technique for extending transport measurements to lower dissipation levels.

\(^{1}\)This work supported by Rowan University
12:03PM B13.00005 Surface plasmon enhancement of fluorescence on gold nanogratings. STEPHANIE WIELE, Department of Physics and Astronomy, Trinity University. IURI GAGNIDZE, Department of Engineering Science, Trinity University. JENNIFER STEELE, Department of Physics and Astronomy, Trinity University — This work focuses on using surface plasmons (SPs) excited on gold wire gratings to enhance the yield from fluorescent molecules. SPs enhance fluorescence by amplifying the electromagnetic near-field that excites the fluorophores as well as providing additional decay channels for the fluorophore. Although it has already been shown that SPs excited on metal nanoparticles can enhance fluorescence, SPs excited on gratings offer several advantages over nanoparticles. Because SPs are excited by the diffraction orders of the grating, changing the angle of incidence of light will change the SP wavelength. The SP excited on the grating can then be tuned on a single plasmonic substrate to overlap the absorption and emission spectrum of many different fluorophores. The ability to tune the SP wavelength through both the absorption and emission wavelength of the fluorophores on a single substrate will give greater insight to how SPs enhance fluorescence and how to maximize the fluorescence enhancement for various biosensing applications.

12:15PM B13.00006 Diffusive Behavior of Lipid Rafts in Multicomponent Membranes. MICHAEL G. LESTER, University of Alabama-Birmingham. MOHAMED LARADJI, University of Memphis. P.S. SUNIL KUMAR, IIT-Madras — The diffusion of nanoscale lipid domains (also known as lipid rafts) in multicomponent membranes in the liquid-liquid coexistence region of the phase diagram is investigated via extensive dissipative particle dynamics simulations. In particular we investigated the effect of membrane diameter and shape (curvature) on the diffusivity of the lipid domains. Our results indicate that the domains exhibit Brownian motion, i.e. the center of mass mean square displacement (\(\Delta R^2\)) = 4Dt, with the diffusion coefficient decreasing as the domain radius, \(r\), is increased. More specifically, we found that \(D \sim 1/r\), i.e. the diffusion of the domains is mainly impeded by viscous drag due to solvent surrounding the membrane. Although the data can also be fitted with the logarithmic expression due to Saffman and Delbrück, the later fit is found to be poorer than that with \(D \sim 1/r\).

1 This work is supported by grants NSF-DMR 0755447 and NSF-DMR 0812470.
2 Saffman and Delbrück, Proc. Nat. Acad. Sci. 72, 3111 (1975)

12:27PM B13.00007 AC Magnetic Susceptibility Probe for Use in a Commercial SQUID Magnetometer. J.D. COHEN, D.M. PAJEROWSKI, M.W. MEISEL, Dept. Physics, Univ. Florida — An AC magnetic susceptibility probe, employing a typical set of mutual inductance coils, has been constructed for operation in a commercial SQUID magnetometer operating down to 1.7 K and up to 7 T. The primary (~1000 turns) and counterwound secondary (each ~1300 turns) coils were wound with 44 AWG Cu wire on a Kapton tube possessing an ID of 6.4 mm. The ensemble of coils is ~30 mm long and has an OD of 8.7 mm, thereby allowing clearance into the sample region of the SQUID magnetometer. One variation of the probe included optical fibers that passed down the center of the stainless steel support rod. The detection electronics involve a lock-in amplifier and the experiment is controlled by LabView software. Typical AC (1 Hz - 1 kHz) fields of ~10 \(\mu\)T afford the study of the temperature, frequency, and dc-field bias dependencies of magnetically interesting samples such as the spin ice material Ho2Ti2O7 [1] and nanoparticles of Prussian blue analogs [2].

1 M. Orendač et al., elsewhere in these proceedings.

12:39PM B13.00008 Recreation of Natural Optical Phenomena. TIFFANY PAONESSA, PETER SHELDON, Randolph College — This project was undertaken to study and fully understand optical atmospheric phenomena. Research was done on the structure and formation of colorful atmospheric phenomena including, but not limited to, primary, secondary, and supernumerary rainbows and halos were created and photographed.

12:51PM B13.00009 Visualization of fracture precursors in vitreous silica: study of under- and over coordinated ions. FRANK JONES, ROMULO OCHOA, DEBORAH KNOX, The College of New Jersey — We have conducted classical molecular dynamics fracture studies of vitreous silica. A new visualization program was designed to observe the fracture process of the sample as a whole. The program also allows users to highlight and focus on the under- and over coordinated oxygen and silicon ions. A BKS potential was utilized to model the ionic interactions. DL-POLY® was the program used to perform simulations. Amorphous silica samples were generated at high temperatures; through a series of quenching and reannealing periods the samples reached room temperature. This method results in samples having, initially, a number of under- and over coordinated ions (less than one percent of all ions) that were randomly distributed. Radial distributions functions were obtained to verify the amorphous structure of the samples. Stress was applied by uniaxially straining the samples at various rates. As a sample was strained there was an increase in under coordinated ions with seemingly no correlation to the region where the sample would break. In all our simulations the under coordinated ions concentrated in the vicinity of the breakage region a few picoseconds before fracture occurred.

1Supported by NSF DMR-0700140 and the UF Scholars Program.

1:03PM B13.00010 Determining the Onset of Amorphization of Crystalline Silicon due to Hypervelocity Impact. C. SHANE POLETTI, MARTINA E. BACHLECHNER, Fairmont State University — Atomic simulations were performed to study a hypervelocity impactor striking a silicon/silicon nitride interface with varying silicon substrate thicknesses. Visualization indicates that the crystalline silicon amorphizes upon impact. The objective of the present study is to determine where the boundary between amorphous and crystalline silicon occurs. In the analysis, the silicon substrate is separated into sixty layers and for each layer the average z displacement is determined. Our results show that the boundary between amorphous and crystalline silicon occurs between layers 20 and 22 for an impactor traveling at 5 km/s. This corresponds to a depth of approximately 32 Angstroms into the silicon. More detailed analyses reveals that the z displacement is noticeably larger for the layers that do not have a silicon atom bonded beneath them compared to the ones that do.

1 Funding for this research project was provided by a WV/NASA Space Grant Scholarship.

1:15PM B13.00011 14N (p,p) Scattering with the KN Van de Graff Accelerator. STEPHANIE LYONS, Randolph College. MICHAEL WIESCHER, University of Notre Dame — The 14N (p,p) scattering experiment was performed with the 4 MV KN Van de Graff Accelerator at the Nuclear Structure Laboratory at the University of Notre Dame. The KN experienced many problems throughout the experiment requiring several belt changes, a change of the drive motor bearings, and a resistor check. The first run of data was converted to cross-sections, and normalized to 30°, which was assumed to be completely Rutherford. Resonances were found at 1.06, 1.55, 1.74, 1.80, 2.34, and 2.47 MeV. These values correlated with previous work done. Further experimentation will be required to clarify the resonances and verify that the scattering at 30° is completely Rutherford.
1:27PM B13.00012 Orientation of the adiabatic demagnetization refrigerator in the Micro-X sounding rocket\textsuperscript{1}, KAITLYN YOHA, Duquesne University, TAREK SAAB, University of Florida, TYLOR WHITMER, PATRICK WIKUS, Kavli Institute for Astrophysics and Space Research, Massachusetts Institute of Technology — The Micro-X sounding rocket is a small rocket equipped with an X-ray telescope and will be launched in 2011. For the telescope to function properly, the adiabatic demagnetization refrigerator (ADR) must be aligned with the optics of the X-ray detectors. During the mission, the ADR will move, thus causing errors. A testing prototype was designed and constructed in the lab to simulate the movement the ADR will experience in flight. This method will monitor the orientation of the ADR relative to the detectors, and allow us to counter the resulting measurement errors.

\textsuperscript{1}This work was supported by NSF REU at the University of Florida, and NASA Grant NNX07AK52G.

1:39PM B13.00013 Use of Multivariate Analysis Techniques to Form a Comparison of Mars Odyssey Gamma Ray Elemental Data to Neutron Data\textsuperscript{1}, PAUL ABBAZIA, Department of Physics and Astronomy, Rowan University — The Lunar Reconnaissance Orbiter’s (LRO) primary mission is exploration. Additional science falls to a secondary focus. LRO does not possess a gamma ray spectrometer, but it has the collimated neutron detector LEND (Lunar Exploration Neutron Detector). It is of interest to determine as much as possible about the moon’s elemental composition using LEND. To do so, data from a similar instrument on Mars Odyssey, HEND (High Energy Neutron Detector), was compared to data from Mars Odyssey’s gamma ray spectrometer (GRS). Elemental maps were previously derived from the GRS data, and a relation to HEND would allow for LEND to fulfill this role on LRO. Toward this purpose, different multivariate analysis techniques were used to compare GRS and HEND data, including Principal Components Analysis (PCA), K-means clustering, and Pearson product-moment correlation. Results indicate that two elements well known to affect neutron counts, hydrogen and iron, can be identified by these techniques. Further analysis may find additional relations, which would have benefits to the fields of geochemistry and neutron spectroscopy.

\textsuperscript{1}This work supported by NASA Goddard Space Flight Center, MUSpIN, SPS.


11:15AM B14.00001 Restricted dislocation mobility in crystals of peanut-shaped colloidal particles, ITAI COHEN, Cornell University — Recent advances in colloidal particle synthesis techniques have enabled the production of a variety of anisotropic yet monodisperse particles, including colloidal “peanuts,” which consist of two connected spherical lobes. Since their shape crudely approximates a dimer, colloidal peanut particles constitute a simple but fundamental extension of the classic system of colloidal spheres. Experimental investigations as well as simulations of colloidal peanut monolayers have shown that at high area fractions the particles form a degenerate crystal (DC). In this structure, the peanut particle lobes order into a triangular lattice, much like close-packed spheres, while the connections between lobe pairs are randomly oriented, uniformly populating the three crystalline directions of the underlying lattice. Comparative studies of crystal formation in rapidly compressed monolayers of peanut-shaped versus spherical particles show that DCs harbor many more defects than equivalent crystals of spheres. This suggests that defect annealing may be frustrated by the constraining rigid connections between particle lobes. To elucidate the interactions between the geometric constraints and defect mobility, we directly examine the mechanisms for dislocation nucleation and propagation in DCs. In particular, we show that obstacles formed by certain particle orientations severely limit the range over which dislocations can glide. Furthermore, we observe that transport over longer distances can proceed through dislocation reactions, which switch the direction of propagation and allow dislocations to bypass such obstacles. In this talk I will discuss the impact that these restricted mechanisms have on the macroscopic properties of DCs.

11:51AM B14.00002 Experimental Study of Brownian Dynamics of Bent-core Colloidal Particles, CHUN-ZHEN FAN, BHUWAN JOSHI, Kent State University, JI-PING HUANG, Fudan University, QI-HUO WEI, Kent State University — Bent-core or banana-shaped molecules exhibit a variety of intriguing liquid crystalline mesophases including nematics and smectic phases. We try to develop suspensions of bent-core shaped colloidal particles to mimic the bent-core liquid crystals. This report will focus on the fabrication of bent-core colloidal particle suspension, and optical microscopic studies of the Brownian dynamics of individual bent-core colloidal particles. The bent-core colloidal particles confined between two glass substrates are observed through dark-field optical microscopy, and their orientation and position are obtained through imaging processing. Results on the translational and rotational Brownian dynamics of these type of particles will be reported.

12:03PM B14.00003 Pinch-off Dynamics of Non-Newtonian Fluids, F. M. HUISMAN, P. TABOREK, University of California Irvine — The pinch-off dynamics of a variety of shear-thinning fluids (foams, concentrated emulsions, and slurries) were studied using high speed videography. The pinch was characterized by the variation of the minimum neck radius rmin as a function of the time to pinch t\(_{\text{p}}\). For inviscid fluids, rmin scales as t\(_{\text{p}}\) to the 2/3 power. We found that for all the shear-thinning fluids rmin scales with t\(_{\text{p}}\) to a power in the range 0.2 to 0.5. To study the transition from conventional inviscid pinch, we systematically varied the concentration of a water-bentonite mixture. As the concentration increased the pinch event transitioned from a needle shape resulting in a satellite drop to a symmetric hyperbolic shape with no satellite drop. These results will be compared with the simulations of Suroy and Basaran (J. Non-Newtonian Fluid Mech. 138 (2006) 134-160).

12:15PM B14.00004 Melting Dynamics of 3D Hard Sphere Colloidal Crystals, DENIZ KAYA, N. L. GREEN, Chemical Engineering Department, C. E. MALONEY, Civil and Environmental Engineering Department , M. WIDOM, Physics Department, M. F. ISLAM, Chemical Engineering; Material Science and Engineering Department, Carnegie Mellon University, Pittsburgh, PA 15213 — We use thermally responsive monodisperse micron sized colloidal particles with hard-sphere interactions to study the melting mechanisms in colloidal crystals. As we increase the temperature, these spherical microgel particles decrease in volume, inducing melting in the colloidal crystals. We use video microscopy and image analysis to determine the dispersion relations and the local elasticity near the melting transition. We compare our findings with existing melting and freezing theories. This work has been partially supported by the NSF through Grants DMR-0619424 and DMR-0645596, and by ACS-PRF.
optical tweezers, rather than a potential landscape as most previous studies use. Changing input power can also change the working direction. Thus we need a state diagram to describe the motor behavior of a colloidal particle in this Brownian motor showed reversible behavior: given input power, working direction changes when particle size grows; given a particle bigger than wavelength trapped in optical tweezers relaxes to equilibrium state. To the contrary, we have found experimentally the particle became a Brownian motor. Furthermore, we have calculated the coupled plasmon modes by a tight-binding approach, taking fully multipolar interactions into account. For approaching particles, the bands can differ significantly from those obtained by the point-dipole approximation due to strong multipolar interaction among the particles. In this regard, Drude metallic spheres and the coupled plasmon modes are calculated in the point-dipole approximation. When the particles approach and finally touch, these modes are characterized by well-defined dispersion relation \( \omega \), resulting in a slow propagation. Thus one can tune the propagation of plasmon modes by simply varying the spacing between the particles. We explore the role of strain in the dynamics of melting and freezing by investigating crystallization on a flat patterned substrate. We find that in comparison with previously performed experiments on flat unpatterned substrates, the dynamics of melting and freezing on such surfaces alter dramatically. For example whereas melting of such crystals on a flat substrate was shown to proceed through an intermediary metastable liquid phase, we find that for surfaces templated with a lattice that is commensurate with that of the melting crystal, this intermediary step is suppressed.

1:03PM B14.00008 Particle Organization by Absorbing State Dynamics, LAURENT CORTÉ, DAVID PINE, P.M. CHAIKIN, Center for Soft Matter Research, NYU — In a recent study we have found that irreversible collisions can lead to a dynamical phase transition between a constantly evolving state and an absorbing, quiescent state where particles self organize to avoid further collisions. Here we investigate the organization and order in the absorbing state in a model where active, overlapping particles are given random displacements. We contrast the order to what is obtained thermodynamically for hard spheres. We also show that correlated displacements between colliding particles can lead to crystallization and suggest that irreversible flows are a different yet effective tool for ordering particles in desired motifs.

1:15PM B14.00009 Diffusion through Colloidal Shells under Stress, J. GUERY, J. BAUDRY, ESPCI, D.A. WEITZ, Harvard, P.M. CHAIKIN, NYU, J. BIBETTE, ESPCI — The permeability of solids has long been associated with a diffusive process involving activated hopping. Tensile stress can affect the activation energy as originally envisioned by Eyring. Here we use liquid core - solid shell, core-shell, solid colloidal particles that are sensitive to osmotic pressure, to follow the permeation of encapsulated probes at various stresses. We unambiguously show that the tensile stress applied on colloidal shells linearly reduces the local energy barrier for diffusion.

1:27PM B14.00100 Dispersion relation and density of states of coupled plasmon modes in periodic chains of metallic nanoparticles, C.W. LING, M.J. ZHENG, K.W. YU, The Chinese University of Hong Kong — Energy transmission through one-dimensional chains of equally spaced metallic nanoparticles has been studied via the propagation of coupled surface-plasmon modes. These modes are characterized by well-defined dispersion relation \( \omega(k) \) and group velocity \( v_g = \frac{\partial \omega}{\partial k} \) in a band. The nanoparticles are routinely modelled by Drude metallic spheres and the coupled plasmon modes are calculated in the point-dipole approximation. When the particles approach and finally touch, these bands can differ significantly from those obtained by the point-dipole approximation due to strong multipolar interaction among the particles. In this regard, we have calculated the coupled plasmon modes by a tight-binding approach, taking fully multipolar interactions into account. For approaching particles, the dipolar bands move from the visible down to the infrared region and \( \omega(k) \) becomes almost independent of \( k \). Concomitantly, the group velocity \( v_g \) showed an intriguing non-monotonic behavior versus the particle spacing. When the spacing decreases, \( v_g \) increases initially but decreases when the particles approach and touch. For moderate spacing, \( v_g \) can be reduced drastically to 0.01, except at \( kd = 0 \) and \( kd = \pi \), resulting in a slow propagation. Thus one can tune the propagation of plasmon modes by simply varying the spacing between the particles.

1:39PM B14.00111 Examining dynamic length scales in a two-dimensional colloidal system, ZACH NADLER, CARA HAGEMAN, VIKRAM PRASAD, ERIC R. WEEKS, Physics Dept., Emory University — We study polystyrene colloids placed at an oil-water interface as a quasi-two-dimensional colloidal system. As the area fraction of the colloidal particles is increased, we see liquid, hexatic, and crystalline phases. The liquid phase is structurally disordered; the hexatic phase has long range orientational order but poor translational order; and the crystalline phase has long range orientational and translational order. We classify these different phases using structural and dynamic parameters from prior work. Using a laser tweezers we trap and drag a particle along the interface and observe its effect on the surrounding colloids. Our interest is in how the response changes near phase transition boundaries, where the ordering of particles can qualitatively change. We characterize the response by the structural defects induced by the dragged particle, as well as the perturbed motion of the surrounding particles. These responses are localized around the dragged particle, and we study how the localization length scale changes with the area fraction of the colloids.

1:51PM B14.00012 State Diagram for Optical Tweezers Induced Brownian Motors, BO SUN, DAVID GRIER, New York University — State Diagram for Optical Tweezers Induced Brownian Motors Bo Sun and David G. Grier Center for Soft Matter Research Department of Physics New York University Optical tweezers are extensively used in physics and biology; most study in literatures assume a colloidal particle trapped in optical tweezers relays to equilibrium state. We have found experimentally the particle became a Brownian motor. Furthermore, this Brownian motor showed reversible behavior: given input power, working direction changes when particle size grows; given a particle bigger than wave length of light, changing input power can also change the working direction. Thus we need a state diagram to describe the motor behavior of a colloidal particle in optical tweezers, rather than a potential landscape as most previous study uses.
11:15AM B15.00001 Walking on water: why your feet get wet. MICHAEL SHELLEY, Courant Institute, New York University, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — Walking on wet pavement during or after heavy rain results in wet shoes, and often, wet feet. We describe a peculiar transport process associated with walking on wet surfaces which results in the vamps, and frequently, the insides, of shoes getting wet. We discuss details of this process and compare experimental results with simple model predictions. Strategies for keeping feet dry will be considered.

11:27AM B15.00002 Breaking beer bottles with cavitation. SUNNY JUNG, Department of Mathematics, MIT, JAKE FONTANA, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, MICHAEL SHELLEY, Courant Institute, New York University — Hitting the top of a beer bottle, nearly full of water, with an open hand can cause the bottle to break, with the bottom separating from upper section. We have studied this phenomenon using a high-speed camera, and observed the formation, coalescence and collapse of bubbles. The breaking of glass is due to cavitation, typically occurring near the bottom edge. We make numerical estimates of the relevant physical parameters, and compare these with experimental observations.

11:39AM B15.00003 Optical Tweezer as a Viscometer1, DANIEL ERENSO, SAMUEL ELROD, TAYLOR BARNES, ANTHONY FARONE, MARY FARONE, Middle Tennessee State University — An optical tweezer (OT) has been widely used to study the mechanical properties of microscopic living biological systems like red blood cells. These studies are based on measurement of deformations caused by a force exerted directly or indirectly by an optical trap. The trap is usually pre-calibrated using Stokes viscous force of the suspension fluids for the biological system which is directly proportional to the viscosity of the fluids. Therefore, calibration of the trap depends on the viscosity of the fluid which depends on temperature. In this work, we have demonstrated that OT can be used to precisely measure the viscosity of biological fluids affected by temperature. Using an infrared laser trap which is calibrated using silica sphere suspended in a distilled deionized water and measuring the power as function of escape velocity, we have measured the viscosities of a newborn and unborn bovine serum with a different concentration of antibodies.

11:51AM B15.00004 Fabrication of a Nanoscale Thermal Anemometry Probe Via Electric Field Assisted Assembly. JASON KAWASAKI, SEAN BAILEY, LEX SMITS, CRAIG ARNOLD, Princeton University — A nanoscale thermal anemometry probe (NSTAP) is being developed to measure instantaneous fluid velocity at ultra-small scales using conventional constant temperature anemometry principles. The probe consists of a 50 nm by 10 um platinum nanowire (NW) suspended between two current carrying electrodes. Previous nanoscale anemometry wires had been fabricated via metal deposition on a photolithography-patterned substrate; however, deposited NWs are not free-standing and thus must later be lifted off the substrate resulting in low process yields. In this presentation, we discuss alternative methods of shrinking the probes further and increasing the yield of successful probes, including growing nanowires from solution to bridge the electrodes, and using dielectrophoresis to align pregrown nanowires between the electrodes. In each of these methods, the NWs are directly shaped near the desired structure eliminating the need for additional processing steps. NSTAP probes manufactured using these methods will also exhibit higher spatial resolution and temporal response than previous NSTAP designs.

12:03PM B15.00005 A Front Tracking Algorithm for Liquid Jet Breakup, WURIGEN BO, JAMES GLIMM, XINGTAO LIU — A numerical study of breakup of a high speed jet is presented using the Front Tracking method in 3D. A robust locally grid based method is applied to handle the topological change of the surface mesh in the simulation, the validation of the method is proved mathematically. Numerical results are presented for 3D simulation of the primary breakup of a liquid jet with turbulent inflow.

12:15PM B15.00006 Coalescence and Pinch-Off in Viscous Liquids1, JOSEPH PAULSEN, University of Chicago, JUSTIN BURTON, Fred Hutchinson Cancer Research Center, SIDNEY NAGEL, University of Chicago — When two fluid drops come into contact, a topological transformation occurs as they rapidly coalesce into a single drop. Because of its speed and geometry, this finite time singularity is difficult to study optically. We therefore use an electrical method to probe viscous coalescence as early as 10 ns after contact. This technique was developed by Burton et al.[1] to study mercury drop pinch-off and adapted for salt-water coalescence by Case et al.[2] revealing a breakdown of the expected universal dynamics in early-time viscous coalescence. For viscous coalescence, we measure a resistance that decreases as t−1 at early times and as t−1/2 at late times, with a crossover time that increases with viscosity. In the inviscid case, these power laws had been interpreted with a model in which the drops coalesce at a slightly deformed interface.


1This work was supported by the Keck Foundation, MRSEC, and NSF

12:27PM B15.00007 Scaling Law for Driven Spreading and Coalescence of Sessile Droplets1, PILGYU KANG, SHAHAB SHOJAEI-ZADEH, CHRISTINE APPLEBY, SHELLEY ANNA, Department of Mechanical Engineering, Carnegie Mellon University, MICRO COMPLEX FLUIDS LABORATORY TEAM2 — This study investigates the dynamics of spreading and coalescence of droplets on a surface, a process important in applications such as inkjet printing, spray coating, and flooding of fuel cells. We use a simple microfluidic device to control the spreading and merging processes. Droplet diameter and maximum height are monitored as functions of time. We compare the dynamics with existing scaling models modified to incorporate time dependent volume, and we extend the model to describe the scaling behavior of the liquid bridge growing between merging droplets on a surface. The experiments agree well with the expected scaling.

1GuSH grant by Graduate Support Programs at Carnegie Mellon University

2Department of Mechanical Engineering, Carnegie Mellon University

12:39PM B15.00008 Temperature profiles near a pinned nucleating bubble, SCOTT PARKER, CHANG-KI MIN, SUNG CHUL BAE, DAVID CAHILL, STEVE GRANICK, University of Illinois — We have measured the temperature distribution on solid surfaces in contact with a nucleating vapor bubble by thermal surface plasmon imaging. Vapor bubbles are created by focused laser heating of an underlying metal substrate. Bubbles are pinned in place by suitable surface functionalization and their shape is characterized by interferometry. Varying the wettability of the surface to control the shape and surface lifetimes of bubbles, we have correlated contact angle, lift-off diameter, and local temperature.
12:51PM B15.00009 Effect of Encapsulated Polymers and Nanoparticles on Deformation of Droplets. O. BERK USTA, University of Pittsburgh, DENNIS PERCHAK, Kodak US Research, ANDREW CLARKE, Kodak European Research, JULIA M. YEOMANS, Oxford University, ANNA C. BALAZS, University of Pittsburgh — We investigate the effects of polymer chains and nanoparticles on the deformation of a droplet in shear and extensional flow using computational modeling: Our model accounts for both the solid and fluid phases explicitly. We show that under shear flow, both the nanoparticles and the encapsulated polymers reduce the shear-induced deformation of the droplet at intermediate capillary numbers; nevertheless, long polymer chains can induce the breakup of the droplet at high capillary numbers. In contrast, under extensional flow we find that the long polymer chains inhibit the breakup and reduce deformation. We study the chain-length and concentration dependence and also present the effects of various parameters such as the wetting strength.

1:03PM B15.00010 Electrorheology Leads to Efficient Combustion. R. TAO, Dept. of Physics, Temple University, K. HUANG, H. TANG, D. BELL, Temple University — Improving engine efficiency and reducing pollutant emissions are important. Since combustion starts at the interface between fuel and air and most harmful emissions come from incomplete burning, reducing the size of fuel droplets for the fuel injection would increase the total surface area to start burning, leading to a cleaner and more efficient engine. While most efforts are focused on ultra-dilute mixtures at extremely high pressure to produce much finer mist of fuel for combustion, the new technology is still under development and only for next generation vehicles. Here we report our fuel injection technology based on new physics principle that proper application of electrorheology can reduce the viscosity of petroleum fuels. A small device is thus introduced just before the fuel injection for the engine, producing a strong electric field to reduce the fuel viscosity, resulting in much smaller fuel droplets in atomization. Both lab tests and road tests confirm our theory and indicate that such a device improves fuel mileage significantly and reduces emission. The technology is expected to have broad applications, applicable to current internal combustion engines and future engines as well. Supported by STWA and RAND.

1:15PM B15.00011 Evolution of Electrified Films on a Porous Inclined Plane. UMA BALAKRISHNAN, University of California Santa Barbara, USHA RANGANATHAN, Indian Institute of Technology Madras — The nonlinear stability of a thin conducting film flow down a porous inclined plane, when an electric field acts normal to the plane is considered. It is assumed that the flow through the porous medium is governed by Darcy’s law and the characteristic length of the pore space is much smaller than the depth of the fluid layer above. Integral Boundary Layer method is employed in obtaining a set of exact averaged equations for the film flow system. Linear stability results through normal mode analysis reveal that the destabilizing influence of the electric field is further enhanced by the porosity of the medium. Critical Reynolds number for the onset of instability decreases with the increase in the permeability of the porous plane. Weakly nonlinear stability analysis using method of multiple scales divulges the existence of zones due to supercritical stability and subcritical instability. Permanent finite-amplitude waves in the supercritical stable region are portrayed by solving the nonlinear evolution equation numerically in a periodic domain. The parameter ranges that support complex nonlinear dynamics is obtained through a combination of theoretical analysis and numerical experiments.

1:27PM B15.00012 Universal cone angle of ac electrosprays due to net charge entrainment. NISHANT CHETWANI, SIDDHARTH MAHESHWARI, H.C. CHANG, University of Notre Dame — The slender meniscus that is obtained by the application of high frequency AC field is quite distinct from DC Taylor Cone. This AC cone shows a continuous longitudinal growth and has much smaller half cone of ~ 11°. Mass spectrometry on the microjet from the AC cone shows that dissociation reaction occurs at the tip but only the low- mobility anionic species are entrained to produce a charged cone. These free negative charges relax to the interface to produce a non-uniform surface charge density that scales with respect to the azimuthal radius as ρ ~ r−2 to balance the singular normal capillary pressure. Repulsion of this entrained surface charge and the Maxwell pressure they induce are estimated with an elliptic integral and a variational formulation produces anormal stress balance with capillary pressure that is only satisfied at a universal angle of 12.6° degrees for the liquids with high dielectric constant in good agreement with the measured values for the organic solvents used in experiments.

1:39PM B15.00013 Impact of Elasticity on Coating Flow near A Moving Contact Line. YULI WEI, STEPHEN GAROFF, Carnegie Mellon University, ENRIQUE RAMÉ, National Center for Space Exploration Research, LYNN WALKER, Carnegie Mellon University — The impact of fluid elasticity and shear thinning on the dynamic wetting of polymer solutions is important because many fluids, even those that are normally considered Newtonian, exhibit non-Newtonian behaviors in the high shear environment of the wedge-like geometry near a moving contact line. Even though this behavior is on the microscopic scale, it has significant impact on wetting on the millimeter scale. Shear thinning dramatically modifies the flow field near a moving contact line and results in a reduced curvature of the free surface. In this talk, we will focus on the effects due to fluid elasticity. Both experimental and numerical results are presented. The fluids we use are the dilute solutions of high molecular weight polyisobutylene (PIB) which exhibit elasticity-dominated rheology with minimal shear thinning. Their wetting behaviors are compared to their oligomer “solvent,” which is considered Newtonian based on standard rheometry. We will also discuss a lubrication analysis of the wedge-like flow field using an Oldroyd-B constitutive relation to mimic the stress evolution of the elastic solution.

1:51PM B15.00014 Field-dependent thermal transfer in magnetic fluids. JUN HUANG, ZHENYU ZHOU, GEOFF HUSTON, WEI LIU, Department of Physics, University of Central Florida — The temperature gradient across a quasi one-dimensional magnetic fluid was measured as a function of the magnetic field and field gradient. It was found that when the field gradient, ∇H, is anti-parallel to the temperature gradient, ∇T, the temperature gradient increases with increasing field and field gradient, but decreases for ∇H parallel to ∇T. For B and ∇H perpendicular to ∇T and gravity, the results are complex and depend on the local configuration of the field and field gradient. We will discuss the results in terms of the effect of local magnetic body force that originates from the local field and the local susceptibility on thermal transfer in magnetic fluids.

2:03PM B15.00015 How does the viscosity of a lubricant effect its tribological behavior? M. AGGLETON, P. TABOREK, University of California, Irvine — The viscosity of many conventional lubricants varies by many orders of magnitude over a small temperature range. We have explored this variation to explore the effect of large viscosity changes on lubrication. We have used a sliding block tribometer to measure the coefficient of friction of a steel-on-steel system with a variety of vacuum compatible hydrocarbon lubricants. Each lubricant was thermally cycled in ultrahigh vacuum from room temperature to below the glass transition temperature. This varies the viscosity without changing the chemistry. Several theoretical models for the temperature dependence of the viscosity of hydrocarbons are applied. The theory described in Cameron (1981) is used to relate the change in viscosity to the coefficient of friction. Some lubricants are found to fit these models up to viscosities as high as 10^6 centiStokes, while for others the model does not even qualitatively describe the data.

This work is supported by Extreme Friction: MURI AFOSR # FA9550-04-1-0381.

Monday, March 16, 2009 11:15AM - 1:15PM — Session B16 DCMP: Cold Fusion —
11:15AM B16.00001 Electrodynamic Component of Pd Electrical Conductivity. MITCHELL SWARTZ. JET Energy, PO Box 81135, Wellesley Hills, MA 02481. — The electrical resistance of Pd in heavy water was found to be significantly lower than in water. This was attributed to the presence of a thin film of hydrogen on the surface of the Pd. The film has a thickness of a few nanometers and its resistance is due to the scattering of conduction electrons by the hydrogen atoms.

11:27AM B16.00002 Study Of The Palladium Hydrogen - Deuterium System. JAN MARWAN. Research and Development, Dr Marwan Chemie, Rudower Chaussee 29, 12489 Berlin, Germany. — Electrochemical deposition of metals from hexagonal isotropic liquid crystal solutions produces metal films with a unique ordered nanostructure in which the cylindrical pores of 1.7 to 3.5 nm run through the film. The pores are separated by a distance of 2.5 nm. The film has a high surface area and a low electrical resistance.

11:39AM B16.00003 Investigation of the Cold Fusion Phenomenon in the Surface Region of Hydrogen Non-occlusive Metal Catalysts; W, Pt, and Au. HIDEO KOZIMA. Cold Fusion Research Laboratory, 597-16 Yatsu, Aoi, Shizuoka, 421-1202, Japan. — In the cold fusion experiments, the following metal catalysts were used: W, Pt, and Au. The experiments showed that the cold fusion reaction occurred in the surface region of the metal catalysts. The reaction was detected by the increase in the electrical resistance of the metal catalysts.

11:51AM B16.00004 Sonofusion: Squeezed Deuteron Clusters, With Small Size, High Energy Density but No High Energy Particles. ROGER STRINGHAM. Firstgate Energies, PO Box 1230 Kilauea, HI 96754. Phone: 808 828 2859. — Sonofusion is a new fusion process that uses ultrasound to squeeze deuteron clusters, which are small and have high energy densities. The clusters are formed in a target by a pulsed laser. The clusters are then squeezed by ultrasound to form a high-energy deuterium plasma.

12:03PM B16.00005 Time-Dependent Changes in Morphology and Composition of Solid Particles Collected from Heavy Water Electrolyte after Electrolysis with a Palladium Cathode. JOHN DASH. Q. WANG, Low Energy Nuclear Laboratory, Portland State University, Portland, OR 97207. — Recent research has developed a technique for imbedding ultra-high density deuterium “clusters” (50 to 100 atoms per cluster) in various metals such as Palladium (Pd), Beryllium (Be) and Lithium (Li). It was found that the condensed matter clusters approach metallic conditions, exhibiting superconducting properties.

12:15PM B16.00006 Study of other methods to increase cluster/dislocation loop densities in electrodes. XIAOLING YANG, GEORGE H. MILEY, University of Illinois, Urbana-Champaign. NPL Associates, Champaign, IL. — Recent research has developed a technique for imbedding ultra-high density deuterium “clusters” (50 to 100 atoms per cluster) in various metals such as Palladium (Pd), Beryllium (Be) and Lithium (Li). It was found that the condensed matter clusters approach metallic conditions, exhibiting superconducting properties.

11:15AM B16.00001 Electrodynamic Component of Pd Electrical Conductivity. MITCHELL SWARTZ, JET Energy, PO Box 81135, Wellesley Hills, MA 02481. — The electrical resistance of Pd in heavy water was found to be significantly lower than in water. This was attributed to the presence of a thin film of hydrogen on the surface of the Pd. The film has a thickness of a few nanometers and its resistance is due to the scattering of conduction electrons by the hydrogen atoms.

We discuss with experimental evidence that $\rho_{Pd}$ has electrodynamic components; some may trigger Lattice Assisted Nuclear Reactions (LANR). Type “B” (anode plate) Pd/D2O/Pt Phusor$^{TM}$ LANR devices (excess heat $\approx$ 175 percent, 1.99 watts) demonstrate two time constants of $\rho_{Pd}(t)$: The first ($< 5$ seconds) is not from deuterium loading. Also, at high loading, Type “B” systems produce an instability oscillation. These possible electrodynamic effects, and the supralinear rise of $\rho_{Pd}$, may trigger, or maintain, LANR.


11:27AM B16.00002 Study Of The Palladium Hydrogen - Deuterium System. JAN MARWAN. Research and Development, Dr Marwan Chemie, Rudower Chaussee 29, 12489 Berlin, Germany. — Electrochemical deposition of metals from hexagonal isotropic liquid crystal phases produces metal films with a unique ordered nanostructure in which the cylindrical pores of 1.7 to 3.5 nm run through the film. The pores are separated by a distance of 2.5 nm. The film has a high surface area and a low electrical resistance.

Electrochemical studies showed that the metal films have a high electroactive surface area with the specific surface area of the order of 91 m$^2$/g. These values together with the TEM and X-ray data are consistent with the expected H$_2$ nanostructure. The hydrogen region of nanostructured Pd in the cyclic voltammetry in 1 M H$_2$SO$_4$ was more resolved than that of plain Pd because of the thin walls of the nanostructure and the high surface area. We could distinguish the hydrogen adsorption and absorption processes. The permeation of hydrogen into the Pd metal lattice occurs with fast kinetics when the Pd surface is blocked by either crystal violet or Pt.


11:39AM B16.00003 Investigation of the Cold Fusion Phenomenon in the Surface Region of Hydrogen Non-occlusive Metal Catalysts; W, Pt, and Au. HIDEO KOZIMA. Cold Fusion Research Laboratory, 597-16 Yatsu, Aoi, Shizuoka, 421-1202, Japan. — There are several experimental data sets showing occurrence of the cold fusion phenomenon (CFP) in such contact metallic catalysts which do not occlude hydrogen isotopes such as tungsten (W), platinum (Pt) and gold (Au). These metals do not occlude hydrogen isotopes and are different from such hydrogen occlusive transition metals usually used in the cold fusion (CF) experiments such as Ti, Ni, and Pd. The non-occlusive isotopes and give us precious information about mechanisms facilitating formation of specific matter for the CFP (CF matter) in the cold fusion material. In the electrolysis experiments with these metals as electrodes and with several electrolytes in light or heavy water, transmuted nuclides were observed in the surface layer of the electrodes. The generated nuclides were localized in areas with a diameter of around a few µm in the surface layer of thickness less than 103 nm. These specific nuclides observed in the host metals, W, Pt and Au, depend on the composition of the electrolyte.

Effects and the "conventional" Coulomb Barrier problem of fusion can be replaced by a considerably richer problem. Infinitely-repeating ordered crystals, to finite crystal lattices, where energy band theory can be re-expressed more precisely through resonant or nearly-resonant quantum mechanics. Talbot Chubb and I have investigated an important problem, relating to extending conventional energy band theory, as it applies to particular, Talbot Chubb and I proposed the idea that deuterium nuclei (deuterons) could occupy energy band states or have overlap with these kinds of states. The reasons for this are related to: 1. Misconceptions, about what was taking place in the experiments, and 2. Limitations of conventional energy band theory. In particular, Talbot Chubb and I suggested that deuterium nuclei could occupy energy band states or have overlap with these kinds of states with "unforeseen" consequences, including, the possibility of nuclear fusion. Conventional energy band theory has limitations, associated with the underlying quantum mechanics. Talbot Chubb and I have investigated an important problem, relating to extending conventional energy band theory, as it applies to infinitely-repeating ordered crystals, to finite crystal lattices, where energy band theory can be re-expressed more precisely through resonant or nearly-resonant effects and the "conventional" Coulomb Barrier problem of fusion can be replaced by a considerably richer problem.

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**Monday, March 16, 2009 11:15AM - 2:15PM – Session B17**

**GQI: Focus Session: Progress towards Scalable Quantum Information Processing**

**318**

**11:15AM B17.00001 ABSTRACT WITHDRAWN**

**11:51AM B17.00002 Electrons on Helium using circuit quantum electrodynamics[1] , DAVID SCHUSTER, Yale University, MARK DYKMAN, Michigan State University, STEPHEN LYON, Princeton University, ROBERT SCHOELKOPF, Yale University** — It is possible to form a two dimensional electron gas at the interface between superfluid helium and vacuum. This unique heterostructure has exceptional bulk properties including electron mobilities exceeding $10^7$ cm$^2$/Vs and electron spin coherence times estimated to exceed 100s. One of the first proposals [2] for quantum computation employed the vertical motional states of electrons on helium but coherent interactions have yet to be realized. I will describe a new proposal [3] which uses a high finesse superconducting transmission line cavity to detect and manipulate the lateral motional and spin states of a single trapped electron on helium. We estimate that it is possible to attain vacuum Rabi frequencies of $g\approx10$ MHz and $T_1\sim T_2\sim1$ ms for the motional state and perhaps even longer coherence times if spin encoding is used.

[3] In preparation

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**12:03PM B17.00003 Simulating electron transport and devices on liquid helium**¹, PASCAL BUGNION, STEPHEN LYON, FORREST BRADBURY, Princeton University — Manipulation of the spin of electrons in surface states on superfluid helium is a promising method for the implementation of a quantum computer. The electrons can be transported around a substrate along channels in a manner analogous to charge-coupled devices. These devices operate on one or a few electrons, which are sufficiently isolated to be treated as classical point charges. The model must therefore incorporate the discreteness of the charges and their interactions, as well as their response to external potentials. These constraints lead towards considering a “molecular” dynamics, multi-electron simulation. The calculation of the electron-electron interactions are complicated by the presence of nearby metallic gates and insulating layers. The concepts necessary for a fast, accurate dynamic simulation of a large collection of individual electrons are elaborated. A computationally cheap approximation of the electrostatic potential due to substrate polarisation for an electron above a channel is proposed. The approximation is compared to an analytic solution. Other substrate geometries which might be used in a quantum computer are also discussed, concentrating on approximations of the potential.

¹P. B. thanks Armourers & Brasier’s Company’s Gauntlet Trust for partial support.
12:15PM B17.00004 Quantum logic with weakly coupled qubits, MICHAEL GELLER, EMILY PRITCHETT, ANDREI GALIAUTDINOV, University of Georgia, JOHN MARTINIS, University of California, Santa Barbara — Effective protocols for performing CNOT quantum logic with qubits coupled by particular high-symmetry (Ising or Heisenberg) interactions are well established. However, many architectures being considered for quantum computation involve qubits or qubits and resonators coupled by more complicated and less symmetric interactions. Here we consider a widely applicable model of weakly but otherwise arbitrarily coupled two-level systems, and use quantum gate design techniques to derive a simple and intuitive CNOT construction. Useful variations and extensions of the solution are given for common special cases.

12:27PM B17.00005 Quantum gates that correct their own (quantum) errors, LORENZA VIOLA, KAVEH KHODJASTEH, Dartmouth College — Scalable quantum computation in realistic devices requires that precise control can be implemented efficiently in the presence of decoherence and operational errors. I will describe a general constructive procedure for designing robust unitary gates on an open quantum system without encoding or measurement overhead. These results allow for a low-level error correction strategy solely based on Hamiltonian engineering using realistic bounded-strength controls, and may prove instrumental to substantially reduce implementation requirements for fault-tolerant quantum computing architectures.

1Work supported by the National Science Foundation under Grant No. PHY-0555417

12:39PM B17.00006 A few-electron triple quantum dot incorporating two fast charge sensors, EDWARD LAIRD, CHARLES MARCUS, Department of Physics, Harvard University, MICA HANSON, ART GOSSARD, Materials Department, University of California at Santa Barbara — A triple quantum dot is defined in a GaAs heterostructure. The occupation of all three dots is monitored using two nearby charge sensing point contacts. Radio frequency multiplexing in a reflectometry setup allows MHz-bandwidth measurements of both charge sensors independently. Configuring the device in the few-electron regime, we achieve coherent spin manipulation using the exchange interaction.

1We acknowledge support from ARO/IARPA, Department of Defense, and Harvard Center for Nanoscale Systems.

12:51PM B17.00007 Interqubit coupling mediated by a high-excitation-energy quantum object, SAHEL ASHHAB, ANTTI NISKANEN, KHALIL HARRABI, YASUNOBU NAKAMURA, THOMAS PICOT, PIETER DE GROOT, KEES HARMANS, HANS MOOI, FRANCO NORI — We consider a system composed of two qubits and a high-excitation-energy quantum object used to mediate coupling between the qubits. After reproducing well-known results concerning the leading term in the mediated coupling, we obtain an expression for the residual coupling between the qubits in the off state. We also analyze the entanglement between the three objects, i.e., the two qubits and the coupler, in the eigenstates of the total Hamiltonian. Although we focus on the application of our results to the recently realized parametric-coupling scheme with two qubits, we also discuss extensions of our results to harmonic-oscillator couplers, couplers that are near resonance with the qubits and multi-qubit systems. In particular, we find that certain errors that are absent for a two-qubit system arise when dealing with multi-qubit systems.

1:03PM B17.00008 Excitons in cavity-embedded quantum dot lattices, MICHAL GROCHOL, CARLO PIERMAROCCI, Department of Physics and Astronomy, Michigan State University — We investigate excitons and trions in a two-dimensional quantum dot lattice embedded in a planar optical cavity. The strong exciton (trion)-photon coupling is described in terms of polariton quasi-particles. First, we focus on Bragg polariton modes obtained by tuning the exciton and the cavity modes into resonance at high symmetry points of the Brillouin zone. The effective mass of these polaritons can be extremely small, of the order of $10^8 m_e$ ($m_e$ is the bare electron mass) and makes them the lightest exciton-like quasi-particle in solids [1]. Second, we consider how disorder affects the properties of Bragg polariton modes. We focus on three kinds of disorder: (i) inhomogeneous exciton energy, (ii) inhomogeneous exciton-photon coupling, and (iii) deviations from an ideal lattice. It is found that in some cases weak disorder increases the light matter coupling and it leads to a larger polariton splitting [2]. Finally, each dot has one electron, and the electron spin determines the polarization of the cavity photon that couples to the dot. Such a “spin lattice” can be used for quantum information processing and we show that by using exciton detuning a conditional phase shift gate with high fidelity can be obtained [3].

1:15PM B17.00009 Low Disorder Si MOSFET Dots for Quantum Computing, E.P. NORDBERG, University of Wisconsin - Madison and Sandia National Laboratories, L.A. TRACY, G.A. TEN EYCK, K. ENG, H.L. STALFORD, K.D. CHILDLS, J. STEVENS, R.K. GRUBBS, M.P. LILLY, Sandia National Laboratories, M.A. ERIKSSON, University of Wisconsin - Madison, M.S. CARROLL, Sandia National Laboratories — Silicon quantum dot based qubits have emerged as an appealing approach to extending the success of GaAs spin based double quantum dot qubits. Research in this field is motivated by the promise of long spin coherence times, and within a MOS system the potential for variable carrier density, very small dot sizes, and CMOS compatibility. In this work, we present results on the fabrication and transport properties of quantum dots in novel double gated Si MOS structures. Coulomb blockade is observed from single quantum dots with extracted charging energies up to an including 5meV. Observed dots were formed both disorder within a quantum point contact, and through disorder free electrostatic confinement. Extracted capacitances, verified with 3D finite element simulations confirm the location of the disorder free dot to be within the designed lithographic structure. Distinctions will be made regarding the effects of feature sizes and sample processing. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

1:27PM B17.00010 Steps toward donor based qubits in Si through integrating single ion Geiger mode avalanche diode detectors, J.A. SEAMONS, E. BIELEJEC, M.S. CARROLL, Sandia National Laboratories — Donor based qubits in Si for solid-state quantum information processing require precise dopant placement into the bulk Si. Placement precision donor is limited by straggle which is strongly dependent upon dopant selection and implantation energy, therefore detection of low energy ions (<10 keV) is desired. Great progress has been made using the combination of a p-i-n diode and electron beam lithography patterned surface mask resulting in a signal to noise limited ~10^3 electron-hole (e-h) pairs detection (D. N. Jamieson et al., Appl. Phys. Lett. 86, 202101 (2005)). We present experimental results for a single ion Geiger mode avalanche diode (SIGMA) detector has been shown to be sensitive to a single 250 keV H+ ion with 100% detection efficiency (J. A. Seamons et al., Appl. Phys. Lett. 93, 40324 (2008)) as well as advances that have been made with the Sigma detector in reducing dark (false) counts by three orders of magnitude and placing an upper bound on the e-h pair sensitivity of ~10^8 produced outside the active region of the SIGMA detector. Future SIGMA designs will enable low energy single ion detection with reduced straggle single donor qubit integration. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.
1:39PM B17.00011 Zeno Quantum Gates in Semiconductor Quantum Dots. KAIJIE XU, YUPIING HUANG, MICHAEL MOORE, CARLO PIERMAROCCHI — Quantum Zeno effect (QZE) is one of the most intriguing quantum phenomena. In the recent literature, there is a series of strongly linked ideas on entanglement generation or computation using the QZE, which have been mainly discussed and explored experimentally in pure quantum optics and superconductors. We propose a scheme for a two-qubit conditional phase gate by QZE with three parallel semiconductor quantum dots [1]. Two of them are charged dots with one additional electron. The spin of these electrons are the logical qubits on which the phase-gate acts. The other dot is an ancillary neutral dot that can perform Rabi oscillations under a resonant laser pulse. With our system setup, we can make use of QZE to gain a π phase shift after a 2π laser pulse depending on the spin configuration in the logical qubits. This phase shift can realize a conditional phase gate. We solve analytically and numerically the master equation with a realistic set of parameters. The result shows that, despite the widely-held belief that decoherence must always be minimized in quantum information processing, in our scheme decoherence can in principle be harnessed to generate high-fidelity gate operation using the QZE. [1] K.J. Xu, Y.P. Huang, M.G. Moore, and C. Piermarocchi, arXiv: 0810.4489 (2008).

1:51PM B17.00012 Large Scale Quantum Computation in a Linear Ion Trap. GUIN-DAR LIN, FOCUS Center and MCTP, Department of Physics, University of Michigan, SHI-LIANG ZHU, South China Normal University, Guangzhou, China, CHRISTOPHER MONROE, JQI and Department of Physics, University of Maryland, LUMING DUAN, FOCUS Center and MCTP, Department of Physics, University of Michigan — Among the approaches to quantum computation, the trapped ion system remains as one of the leading candidates. The linear Paul trap provides the most convenient architecture for quantum gate operations over a few ions, and the basic requirements for quantum computation have been demonstrated in this setup. However, scaling up this system to a large number of qubits so far remains a formidable challenge because of several obstacles, including the instability of the linear structure and the difficulties of the sidemode cooling and addressing for a large ion array. The recent approach to scalable ion trap computation thus has to use a more complicated architecture where the ions are shuttled over different trapping regions. Here, we propose a way to implement large-scale quantum computation in a linear trap by overcoming all the theoretical obstacles. Through excitation of the transverse photon modes in an anharmonic trap, we show that high-fidelity quantum gates can be achieved on ions in a large linear architecture under the Doppler temperature without the requirement of sidemode resolving.

Monday, March 16, 2009 11:15AM - 2:15PM Session B18 DPOLY: Focus Session: Templated Assembly of Polymers 319

11:15AM B18.00001 Directed Assembly of Biological Polymers. ALINE MILLER, University of Manchester — The self-assembly of polypeptides into beta-sheet rich nanofibrils has attracted considerable attention in recent years to both understand amyloidogenesis and for their potential biomaterials applications. This self-assembly process is generic to all proteins where fibrillation is typically induced under harsh conditions of low pH and/or high temperature, which are of course not suitable for biomaterials applications. Here we will outline the method developed in our laboratory to create thermo-reversible fibrillar hydrogels from aqueous solutions of a series of proteins by adding a reductant. Proteins studied include beta-lactoglobulin, ovalbumin, lysozyme and bovine serum albumin; all contain an increasing number of disulfide bridges that are disrupted by the reductant. Such disruption destabilises the native state of the protein and this allows us to form transparent, self-supporting hydrogels under physiological conditions. The potential to control and manipulate the gel properties, including mechanical strength and structure (fibre diameter and mesh size of hydrogel) has been explored by varying the protein (consequently the number of disulfide bridges), protein concentration, reductant concentration and ionic strength of the matrix. Our results will be presented here and similarities and differences highlighted. Furthermore we will present both our 2- and 3-dimensional cell culture experiments that show the gel matrix promotes both fibroblast and chondrocyte cell spreading, attachment and proliferation; indicating our hydrogels are biocompatible and they can provide a viable support for different cell types.

11:51AM B18.00002 Hydroxyapatite growth induced by self-assembled noncollagenous extracellular protein: a study on biomineralization in vitro. XIAOLAN BA, YIZHI MENG, NADINE PERNODET, SUE WIIRICK, CHRIS JACOBSEN, Stony Brook University, HELGA FUREDI-MILHOFER, The Hebrew University, YI-XIAN QIN, MIRIAM RAFAILOVICH, Stony Brook University, ELAINE DIMASI, Brookhaven National Laboratory — It is known that the role of various ECM proteins in the formation of calcium phosphate during the biomineralization. Here we will introduce the calcium phosphate mineralization process in vitro using two different ECM proteins, fibronectin and elastin. The mechanical properties of the protein fibers during the early stages were probed by shear mode force microscopy. The development of the mineral crystals along the protein matrices was investigated by scanning electron microscopy, soft x-ray scanning transmission microscopcopy, and grazing-incidence synchrotron x-ray diffraction. The elastic modulus of the fibers in the elastin-fibronectin mixture increased to a greater extent than that of the fibers from a single protein. In the presence of fibronectin, longer exposure in the mineral solutions led to the formation of hydroxyapatite crystals templated along the self-assembled fiber structures, while elastin fibers collected calcium without crystallizing. Ca L-edge XANES spectra confirm that Ca in the Ca-elastin complex lacks the mineral anion coordination found in the fibronectin systems and in Ca mineral controls.

12:03PM B18.00003 Replication of Optical Microstructures of Papilio palinurus through Biomimicry. MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, MATIJA CRNE, School of Chemistry and Biochemistry, Georgia Institute of Technology, VIVEK SHARMA, Department of Mechanical Engineering, Massachusetts Institute of Technology, JOHN BLAIR, School of Material Science and Engineering, Georgia Institute of Technology, JUNG OK PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, CHRISTOPHER J. SUMMERS, School of Material Science and Engineering, Georgia Institute of Technology — The coloration of animals in nature is sometimes based on their structure rather than pigments. Structural coloration based on diffraction, multilayer reflection, cholesteric analogues or photonic crystal-like structures is pervasive especially in the world of insects. The color of Papilio palinurus results from microbowl lined with a multilayer of air and chitin. The green color is the result of color mixing of the yellow light reflecting from the bottom of the bowl and the blue light reflecting from the sides of the bowl. We have used breath figure templated assembly as the starting point to mimic the structure of Papilio palinurus. We were able to produce microbowl which were then coated with a multilayer of alternating titanium oxide and aluminum oxide. The resulting structure exhibits the same color mixing as the original butterfly structure does.
12:15PM B18.00004 Polyelectrolyte and nanoparticle adsorption to nanopatterned surfaces, THUY CHASTEK, STEVEN HUDSON, VINCE HACKLEY, NIST, Gaithersburg, MD 20899 — The adsorption of polyelectrolytes and nanoparticles onto patterned and curved surfaces is investigated (by fluorescence and electron microscopy) and exploited to produce anisotropic patchy particles. Various anisotropic properties are necessary for the self-assembly of complex structures. In this work, particles were bound temporarily to a substrate, so that part of their surfaces is occluded during subsequent surface modification by the adsorption of polyelectrolyte. The substrate surface charge has a significant effect on the adsorption of particles, which is achieved in a novel way in comparison to bare glass substrates. These include much reduced deposition time, a high degree of coverage, and the ability to accommodate both negatively and positively charged particles. Moreover, patch production yield is consistently 99 ± 1%. Rapid coating methods transferable to roll-to-roll processing were tested, and step-by-step characterization methods to evaluate yield were developed. High-yield site-specific binding of complementary spheres to the lithographic region of patchy particles and surfaces was demonstrated, including binding to positive and negative patches.

12:27PM B18.00005 Vertical Alignment of Single Wall Carbon Nanotubes (SWNTs) in Thin Polymer Films, MEAGAN MAUTER, MENACHEM ELIMELECH, CHINEDUM OSUJI, Yale University — Thin polymer films (1-10 um) incorporating singly dispersed, vertically aligned carbon nanotubes have a diverse set of potential applications. Desalination membranes that use aligned SWNT as pores, for instance, are predicted to exhibit high flux and salt rejection through size exclusion of hydrated ions. Current fabrication techniques, however, are unable to realize the vertical assembly of narrow diameter SWNTs. Here, we direct the vertical alignment of SWNTs in thin films by using magnetic field aligned lyotropic surfactant mesophases as structure directing templates. The short alkyl tails of the surfactant impart negative diamagnetic anisotropy to worm-like micelles and lead to parallel alignment of the liquid crystalline (LC) director in an applied magnetic field. The nanotubes orient preferentially with their long axis parallel to the director field of the mesophase, thus promoting their vertical alignment in the system. The LC mesophase incorporates monomers that are polymerized by UV exposure after nanotube alignment to form the polymer matrix. X-ray scattering and optical spectroscopy are used to characterize the field-guided assembly process. The present system may have additional applications for polymer reinforcement using carbon nanotubes.

12:39PM B18.00006 STM study of stereoselective oligomeric chains on cobalt oxide templates, DAEJIN EOM, HUI ZHOU, KWANG T. RIM, MICHAEL LEFENFELD, COLIN NUCKOLLS, GEORGE W. FLYNN, TONY F. HEINZ, Columbia University — Stereoselective oligomeric chains of cis-1,4-poly(2,3-dimethyl-1,3-butadiene) have been grown using the cobalt oxide surface as a template. The chains were formed by vacuum deposition of the monomer on an oxidized Co(0001) surface held at room temperature. The geometric structure of the 1-dimensional chains and their relationships to the structure of the surface were probed using scanning tunneling microscopy (STM). The typical chains were more than 10 monomer units in length and were highly linear in structure. When the chains were annealed to a temperature of 480 K, however, their morphology abruptly changed to irregularly shaped curves. We interpret this transformation as the result of scission of the methyl side groups of the oligomers. In addition to comprehensive STM topography data, we have investigated the chains using scanning tunneling spectroscopy (STS). The STS spectra show features with an energy spacing of 0.17 eV. We interpret this response as arising from an inelastic tunneling channel involving excitation of the symmetric deformation mode of the methyl side groups.

12:51PM B18.00007 Breath-figure-templated assembly of holey polymer films1, VIVEK SHARMA, Hatsopoulos Microfluids Laboratory (HML), Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge MA 02139., MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA 30332. — Breath figures formed on evaporating polymer solutions exposed to the blast of humid air involve growth and self-assembly of water drops that are non-coalescent. The hexagonally close packed, nearly monodisperse drops, eventually evaporate away, leaving a polymer film with ordered array of pores. We provide the first quantitatively correct simulation of the elucidation of the mechanism of this breath-figure-templated assembly. The dynamics of drop nucleation, growth, and coalescence and self-assembly are modeled by accounting for various transport and thermodynamic processes. The theoretical framework developed in this study allows one to rationalize and predict the structure and size of pores formed in different polymer-solvent systems under given airflow conditions.

1>Funded by NSF-DMR

1:03PM B18.00008 Gelation in Semiflexible Polymers1, VENKAT PADMANABHAN, SANAT K. KUMAR, Columbia University — Discrete Molecular Dynamics/Collision Dynamics has been employed to study the formation of a physical gel by semi-flexible polymer chains. The formation of a geometrically connected network of bundles of chains is investigated as a function of temperature. As the temperature is lowered, a percolated homogeneous solution phase separates to form a non-percolated nematic fluid and upon further decrease in the temperature, it goes back to a percolated gel state. The gelation, at lower temperatures, is due to the dynamic arrest of chains, preventing them from completing the phase separation process. The cooling rate also plays an important role in deciding the final outcome. Quenching the system, to the final temperature, at a faster rate yields gelation while slower quenches result in phase separation.

1>DOE

1:15PM B18.00009 Highly Ordered Block Copolymer Templates for the Generation of Nanos-structured Materials, E. BOJHE GOWD, BHANU NANDAN, NADJA C. BIGALL, ALEXANDER EYCHMULLER, MANFRED STAMM, LEIBNIZ INSTITUTE OF POLYMER RESEARCH DRESDEN, HOHE STRASSE 6, 01069 DRESDEN, GERMANY TEAM — Among many different types of self-assembled materials, block copolymers have attracted immense interest for applications in nanotechnology. Block copolymer thin film can be used as a template for patterning of hard inorganic materials such as metal nanoparticles. In the present work, we demonstrate a new approach to fabricate highly ordered arrays of nanoscopic inorganic dots and wires using switchable block copolymer thin films. Various inorganic nanoparticles from a simple aqueous solution were directly deposited on the surface reconstructed block copolymer templates. The preferential interaction of the nanoparticles with one of the blocks is mainly responsible for the lateral distribution of the nanoparticles in addition to the capillary forces. Subsequent stabilization by UV-irradiation following by pyrolysis in air at 450 °C removes the polymer to produce highly ordered metallic nanodot structures. This method is highly versatile as the procedure used here is simple, eco-friendly and provides a facile approach to fabricate a broad range of nanoscaled architectures with tunable lateral spacing.

1:27PM B18.00010 Polymeric nanocomposite comprising size-controlled organic nanostructures via copolymer-directed self-assembly, DEQUAN XIAO1, KUNHUA LIN, Department of Chemistry, Sichuan University, Chengdu, 610064 China, QIANG FU, Department of Polymer Science and Engineering, Sichuan University, State Key Laboratory of Polymer Materials Engineering, Chengdu, 610065 China, QINJIAN YIN, Department of Chemistry, Sichuan University, Chengdu, 610064 China — Inspired by inorganic nanomaterials, low-dimensional organic nanostructures have emerged as a new field of nanomaterials with the presence of size-dependent physical properties. Here, we report a polymeric nanocomposite comprising size-controlled organic nanostructures, formed by copolymer-directed self-assembly. By TEM and SEM images, we found the near-spherical shapes of the zero-dimensional organic nanoparticles. A strongly broadened Raman shift band was probed, suggesting the presence of size-dependent quantum confinement effect. By proof-of-principle quantum chemical calculations, we further explain that the strong Raman broadening is caused by the heterogeneous size-distribution of the organic nanoparticles. The present polymeric nanocomposite opens a new route for exploring low-dimensional organic nanostructures with size-dependent physical properties.

1>current address: Department of Chemistry, Duke University, Durham, NC 27708
1:39PM B18.00011 Orientational Change of Microphase-Separated Domains of Block Copolymer Thin Films Placed on Ordered Nanoparticle Monolayers. KOOKHEON CHAR, TAEHEE KIM, Seoul National University — Orientation of microphase-separated domains of diblock copolymer (BCP) thin films deposited on ordered nanoparticle (NP) monolayers was investigated. Ordered NP monolayers were prepared on silicon substrates with the Langmuir-Blodgett deposition technique. Parallel orientation of anisotropic microdomains (cylinders and lamellae) of BCP thin films with respect to the substrate is preferred on bare silicon substrates due to the preferential enthalpic interaction with one of BCP blocks, while the perpendicular orientation is preferred on the lattice-like ordered NP monolayers due to the roughness induced from the NP monolayers which can exert elastic deformation on the parallel-oriented microdomains, suppressing the substrate-induced parallel orientation. The effects of NP size as well as BCP film thickness on the orientation of BCP domains were systematically studied with AFM and Grazing Incidence Small-Angle X-ray Scattering (GISAXS). The rectification of perpendicularly oriented BCP microdomains onto underlying NP lattices was analyzed with SEM for thin BCP films (less than 100 nm in thickness). With this experimental technique, we observed the persisted perpendicular orientation of BCP microdomains on NP vacant sites up to the width of NP vacant sites less than 290 nm (∼11 Lₐ).

1:51PM B18.00012 Directed self-assembly of block copolymers for resolution enhancement and pattern rectification. JOY CHENG, CHARLES RETTTNER, DANIEL SANDERS, ALSHAKIM NELSON, HOA TRUONG, HO-CHEOL KIM, WILLIAM HINSBERG, SELF-ASSEMBLY TEAM — Directed polymer self-assembly which combines lithographically defined substrates and self-assembled polymers has been considered as a potential candidate to extend conventional lithography techniques. Self-assembled block copolymer domains can multiply the spatial frequency and improve pattern quality of the underlying resist prepattern. Lamella-forming PS-b-PDMAEMA is spin-coated on patterned substrate with alternating stripes of resist/neutral underlayer and annealed to generate well-aligned microdomains. The performance of directed self-assembly depends on the pitch of resist prepattern and resist pattern quality. For linear line-space pattern, defect-free frequency doubling can be achieved within ±5% mismatch between periodicity of block copolymers and pitch of resist patterns. Less mismatch tolerance was observed in concentric circular pattern. The self-healing capability of block copolymers has been explored by inducing dotted resist lines. Pattern rectification and frequency multipication can be successfully achieved when sufficient local spatial information is given in the resist prepattern.

2:03PM B18.00013 Tetragonal Ordering in Block Copolymer-Homopolymer Blend Films Laterally Confined in a Square Well. SU-MI HUR, CARLOS GARCIA-CERVERA, ED KRAMER, GLENN FREDRICKSON, UC BERKELEY — Self-consistent field theory (SCFT) simulations are presented for a melt blend of AB diblock copolymers and A homopolymers in a thin film confined to a square well. The work aims to guide self-assembly towards tetragonal ordering, which is a pattern of technological interest in block copolymer lithography. By using a system of A homopolymers and PS-b-PEO diblock copolymers, we have been able to observe hexagonal and body-centered cubic structures in block copolymer films. A phase diagram is presented that shows the region of stability of the tetragonal phase as a function of chain length and volume fraction of the homopolymer additive, in addition to several other interesting phases that result from a competition between surface and bulk contributions to the free energy. Results are also presented on the effect of line edge roughness in the square confinement well on the achievement of robust and defect free tetragonal order.

Monday, March 16, 2009 11:15AM - 2:03PM — Session B19 DPOLY: Focus Session: Polymers and Ionic Liquids

11:15AM B19.00001 Block Copolymers and Ionic Liquids: A New Class of Functional Nanocomposites. TIMOTHY LODGE, University of Minnesota — Block copolymers provide a remarkably versatile platform for achieving desired nanostructures by self-assembly, with length scales varying from a few nanometers up to several hundred nanometers. Ionic liquids are an emerging class of solvents, with an appealing set of physical attributes. These include negligible vapor pressure, high chemical and thermal stability, tunable solvation properties, high ionic conductivity, and wide electrochemical windows. For various applications it will be necessary to solidify the ionic liquid into coexisting phases, such as microemulsions and micelles. One example includes formation of spherical, cylindrical, and vesicular micelles by poly(butadiene-b-ethylene oxide) and poly(styrene-b-methylmethacrylate) in the common hydrophobic ionic liquids [BMIM][PF₆] and [EMI][TFSI]. This work has been extended to the formation of reversible micelle shuttles between ionic liquids and water, whereby entire micelles transfer from one phase to the other, reversibly, depending on temperature and solvent quality. Formation of ion gels has been achieved by self-assembly of poly(styrene-b-ethylene oxide-b-styrene) triblocks in ionic liquids, and by the thermoreversible system poly(N-isopropylacrylamide-b-ethylene oxide-b-N-isopropylacrylamide), using as little as 4% copolymer. Further, these gels have been shown to be remarkably effective as gate dielectrics in organic thin film transistors. The remarkably high capacitance of the ion gels (≥10 µF/cm²) supports a very high carrier density in an organic semiconductor such as poly(3-hexylthiophene), leading to milliamp currents for low applied voltages. Furthermore, the rapid mobility of the ions enables switching speeds approaching 10 kHz, orders of magnitude higher than achievable with other polymer-based dielectric systems such as PEO/LiClO₄. Finally, we have shown that ordered nanostructures of block copolymers plus ionic liquids show the characteristic self-assembly properties of strongly-segregated systems. Prospects for anisotropic ionic conductivity are also being explored.

1 Supported by the National Science Foundation

11:51AM B19.00002 Phase Behavior of Block Copolymer Solutions in an Ionic Liquid. J.M. VIRGILI, M.L. HOAFRCOST, N.P. BALSARA, R.A. SEGALMAN, UC Berkeley — Incorporation of ionic liquids into block copolymers is of interest for applications such as high temperature fuel cell membranes. We investigate the lyotropic and thermotropic phase behavior of solutions of poly(styrene-b-2-vinyl pyridine) (S2VP) block copolymers in an ionic liquid consisting of imidazole and bis(trifluoromethane)sulfonamide (HTFSI). This work has been extended to the formation of reversible micelle shuttles between ionic liquids and water, whereby entire micelles transfer from one phase to the other, reversibly, depending on temperature and solvent quality. Formation of ion gels has been achieved by self-assembly of poly(styrene-b-ethylene oxide-b-styrene) triblocks in ionic liquids, and by the thermoreversible system poly(N-isopropylacrylamide-b-ethylene oxide-b-N-isopropylacrylamide), using as little as 4% copolymer. Further, these gels have been shown to be remarkably effective as gate dielectrics in organic thin film transistors. The remarkably high capacitance of the ion gels (≥10 µF/cm²) supports a very high carrier density in an organic semiconductor such as poly(3-hexylthiophene), leading to milliamp currents for low applied voltages. Furthermore, the rapid mobility of the ions enables switching speeds approaching 10 kHz, orders of magnitude higher than achievable with other polymer-based dielectric systems such as PEO/LiClO₄. Finally, we have shown that ordered nanostructures of block copolymers plus ionic liquids show the characteristic self-assembly properties of strongly-segregated systems. Prospects for anisotropic ionic conductivity are also being explored.

12:03PM B19.00003 Ordering of Triblock Copolymer Surfactants by Blending with a Room Temperature Ionic Liquid. DANIEL MIRANDA, JAMES WATKINS, THOMAS RUSSELL, University of Massachusetts Amherst — Well-ordered block copolymer microdomains were obtained by blending Pluronic® PEO-PPG-PEO triblock copolymer surfactants with the room temperature ionic liquid 1-butyl-3-methylimidazolium bis(trifluoromethane)sulfonimide. The selective association of the ionic liquid with the PEO blocks increases the segregation strength by increasing the effective interaction parameter between the blocks. The next copolymer is phase-mixed in the melt whereas the addition of ionic liquid to the copolymer results in phase segregation, forming well-ordered microdomains. The ionic liquid was confirmed to interact with the PEO blocks by a depression in the melting point of the blends with increasing ionic liquid concentration. Further, small angle x-ray scattering experiments show a decrease in the breadth of the first order peak, as well as the appearance of higher order peaks, with increasing ionic liquid concentration. These results confirm the formation of well-ordered microdomains.

3 MRSEC, CHM
12:15PM B19.00004 Phase separation induced by polymer-ionic molecule complexation. ISSEI NAKAMURA, AN-CHANG SHI, McMaster University — The miscibility of polymers in ionic solutions has attracted long-standing interest in polymer science. In particular, it has been demonstrated experimentally that phase separation can be driven by complexation of polymers and ionic-molecules. Thermally reversible strong forces such as hydrogen bonding and electrostatic force are often employed to induce the complexation. In this study, we developed a self consistent field theory for polymers which are capable of binding small ionic molecules. Specifically, poly(vinyl alcohol) and borate ion in aqueous solution with sodium chloride are used as a model system. Binding isotherm, phase diagrams, as well as comparisons with experiments, will be presented. The theory provides a closed-loop region for an instability of the homogeneous phase in the phase diagram. Implications of our results to the sol-gel transition arising from the correlation between unoccupied and occupied ion-binding sites of polymers are discussed.

12:27PM B19.00005 Morphology and Ion Transport in Mixtures of Polymers and Ionic Liquid, JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6272, LIANG GWEE, YOSSEF A. ELABD, Department of Chemical and Biological Engineering, Drexel University, Philadelphia, PA 19104, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia 19104-6272 — Mixtures of polymers and ionic liquid have been prepared using homopolymers, random copolymers, and block copolymers: poly(methyl methacrylate), poly(methyl methacrylate-ran-styrene), and poly(methyl methacrylate-b-styrene). The ionic liquid is 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide. These mixtures are investigated using X-ray scattering and electron microscopy. Mixtures of the homopolymer and random copolymer with the ionic liquid are homogeneous and amorphous morphology with excess scattering as content of ionic liquid increases. The block copolymer and ionic liquid mixtures show ordered structures typical of block copolymers that vary with ionic liquid content. The morphologies of the copolymer-ionic liquid mixtures can be correlated with the conductivities.

12:39PM B19.00006 Dissolving Polymers in Ionic Liquids. DAVID HOAGLAND, JOHN HARNER, Univ. of Massachusetts Amherst — Dissolution and phase behavior of polymers in ionic liquids have been assessed by solution characterization techniques such as intrinsic viscosity and light scattering (static and dynamic). Elevated viscosity proved the greatest obstacle. As yet, whether principles standard to conventional polymer solutions apply to ionic liquid solutions is uncertain, especially for polymers such as polyethylene and hydrophobic block copolymers that may specifically interact with ionic liquid anions or cations. For flexible polyelectrolytes (polymers releasing counterions into high dielectric solvents), characterization in ionic liquids suggests behaviors more typical of neutral polymer. Coil sizes and conformations are approximately the same as in aqueous buffer. Further, several globular proteins dissolve in a hydrophilic ionic liquid with conformations analogous to those in buffer. General principles of solubility, however, remain unclear, making predictions of which polymer dissolves in which ionic liquid difficult; several otherwise intractable polymers (e.g., cellulose, polyvinyl alcohol) dissolve and can be efficiently functionalized in ionic liquids.

12:51PM B19.00007 Polyester Spherulite Crystallization in Ionic Liquids. KATHY SINGFIELD, SHAWNA MITCHELL, Saint Mary’s University — A series of polyesters have been crystallized in ionic liquids. Spherulites of the polyesters have been grown isothermally from different ionic liquids after cooling the single phase polymer/ionic liquid system from above the polymer melting point temperature. To the authors’ best knowledge this is the first reported account of polyester spherulites grown from these non-traditional solvents. The combination of physical properties of the crystallizing system supports the un-restrained branching/splitting volume-filling growth in all radial directions of the suspended crystallizing entity. The morphology of the collected spherulites at various stages of their formation was examined using scanning electron microscopy (SEM). The SEM results provide a clear visual inspection of the early-stage growth forms and the branching/splitting patterns involved in their evolution to the final spherical form.

1:03PM B19.00008 Understanding Ion Transport in Polymerized Ionic Liquids using Dielectric Spectroscopy. U. HYEOK CHOI, Penn State University, HONG CHEN, Drexel University, WENJUAN LIU, Penn State University, YOSSEF A. ELABD, Drexel University, RALPH H. COLBY, Penn State University — In order to deduce the mechanism of ion conduction in ion-containing polymers, not only the conductivity needs to be measured but also the number density and mobility of conducting ions must be determined using broadband dielectric spectroscopy, covering broad frequency and temperature ranges. To obtain a transference number of unity, one ionic charge is covalently bonded to the polymer so that only the counterions can contribute to ion conduction. In this study, imidazolium-containing monomer was synthesized and polymerized to make a cationic homopolymer with either tetrafluoroborate or bis(trifluoromethanesulfonfyl)imide anionic counterions. These ions can associate into pairs and larger aggregates. The degree of ion pairing can be estimated from the temperature dependence of the dielectric constant and knowledge of the dipole moment of the ion pair, using the 1936 Onsager equation. Using the 1953 Macdonald model makes it possible to determine concentration and mobility of mobile counterions from analysis of electrode polarization in dielectric spectroscopy.

1:15PM B19.00009 Enhanced ionic conductivity of polyurethane ionomers by self-solvating cations. SHIH-WA WANG, RALPH COLBY, Pennsylvania State University — We study the effect of different cations on ionic conductivity and dielectric properties of polyurethane ionomeric single-ion conductors with para-phenyl diisocyanate and anionic diols (carboxylate or phosphonate) constituting the hard segments and poly(ethylene glycol) as the soft segment. Bulky cations such as tetra-alkyl ammonium can increase ionic conductivity compared to metallic polyurethane ionomers. We show that the presence of ether oxygen on conducting cations even more, ether oxygens, which are well-known to solvate cations, are incorporated in the alkyl tail of ammonium-type cations. By comparing segments and poly(ethylene glycol) as the soft segment. Bulky cations such as tetra-alkyl ammonium can increase ionic conductivity compared to metallic polyurethane ionomers.
1:39PM B19.00011 Processing of Natural Polymer-nanocomposites using Ionic Liquids as “Green Solvents”, SAMEER RAHATEKAR, NIST, ASIF RASHEED, FDA, RAVUL JAIN, Georgia Tech, K. KOZIOL, ALAN WINDLE, University of Cambridge, PAUL TRULOVE, US Naval Academy, SATISH KUMAR, Georgia Tech, JEFFREY GILMAN, NIST, NIST COLLABORATION, GEORGIA TECH COLLABORATION, UNIVERSITY OF CAMBRIDGE COLLABORATION — We report fiber spinning of natural polymers such as cellulose and silk using ionic liquids. Ionic liquids can dissolve cellulose and silk and are less hazardous that the traditional solvents used for dissolving cellulose. We use imidazolium based ionic liquids as a common solvent to process natural polymers and carbon nanotubes. Cellulose/carbon nanotubes based fibers are spun using wet spinning process. The rheological, mechanical thermal and electrical properties of the fibers are measured. We also characterize the cellulose nanocomposites fibers using ionic liquids by SEM/TEM, X-ray diffraction, TGA and FTIR analysis. Silk and carbon nanotubes fiber processing is also reported using ionic liquids as process. The rheological, mechanical thermal and electrical properties of the fibers are measured. We also characterize the cellulose nanocomposites fibers using ionic liquids by SEM/TEM, X-ray diffraction, TGA and FTIR analysis. Silk and carbon nanotubes fiber processing is also reported using ionic liquids as common solvent.

1:51PM B19.00012 Biocompatible Ionic Liquid-Derived Conducting Polymers\(^1\), MILLICENT FIRESTONE, CHRISTOPHER BURNS, SUNGWON LEE, Argonne National Laboratory — A significant and frequently encountered challenge when making an electrical connection to a protein is that its electron-transfer sites are buried within the polypeptide matrix and thus, are not readily accessible to bulk metal electrodes. A further complicating factor is that inorganic (i.e., metallic) electrodes are often incompatible with biological samples. These obstacles might be overcome by the use of conducting oligomers and / or polymers, which are flexible, offering a means to access remote redox centers. These oligomers can be readily modified to include chemical moieties that can connect covalently to sites near redox centers. In addition, conducting polymers can be made to be environmentally responsive (dynamic), processable (conformal coating, soluble) and mechanically durable, thus enabling them to function as an electrical conduit (wire or electrode) to biomolecules. In this work, we describe the design, synthesis and electrochemical properties of thiophene-based ionic liquid monomers and their bulk polymerization by chemical oxidation to yield cationic, aqueous-soluble polymers. Preliminary studies evaluating the electropolymerization of these monomers into nanostructured thin films will also be presented.

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\(^1\)This work was performed under the auspices of the Office of BES, DMS, US-DOE, under contract No. DE-AC02-06CH11357.

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11:15AM B20.00001 Polymers for new battery technologies., MOHIT SINGH, Seeo Inc — The chemical and electrochemical reactivity of the components comprising today’s lithium batteries has severely limited their lifetime and stability, and attempts to push the limits on energy density have exacerbated these stability issues. The weakest link in terms of safety and stability of Li ion systems is the organic liquid electrolyte that facilitates the Li\(^+\) ion transport between the electrodes. The electrolyte is flammable and electrochemically unstable against the graphitic anode. It is the continuous electrochemical degradation of the electrolyte at the electrodes that leads to poor cycle life of the batteries, and in some cases runaway reactions that lead to explosions. Dry polymer electrolytes alleviate the electrochemical stability problem by offering a stable electrode-electrolyte interface. The absence of flammable liquids prevents runaway reactions. The main hurdle that has prevented dry polymer electrolytes from being commercialized is low ionic conductivity, and challenges in interfacing with the electrode materials. We demonstrate a novel approach towards addressing these challenges that renders batteries with excellent cycle lives, and thermal stability.

11:51AM B20.00002 Control of Domain Orientation in Block Copolymer Electrolyte Membranes at the Interface with Humid Air, MOON JEONG PARK, SUHAN KIM, ANDREW M. MINOR, NITASH P. BALSARA, Department of Chemical Engineering, Materials Sciences Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, USA — Access to ion transporting channels in polymer electrolyte membranes depends crucially on the orientation of hydrophobic and hydrophilic domains at the surface. We demonstrate that domain orientation of polymer electrolyte membranes made from polystyrenesulfonate-b-methoxy(polyethylene) (PS-PMO) copolymers can be tuned by controlling sulfonation level and moisture content of the air. At low sulfonation levels, highly ordered hydrophobic PMO cylinders oriented perpendicular to the film surface are obtained, when the film is contacted with humid air. Increasing the sulfonation level results in a transition from perpendicular to parallel orientation. Our conclusion is based on three-dimensional characterization of membranes using electron microscopy of samples prepared by the shadow focused ion beam technique, grazing incident small angle x-ray scattering, and electron tomography.

12:03PM B20.00003 Vertical phase-separation due to differences in surface energies in bulk heterojunction polymer solar cells, SARAH COWAN, ANSHUMAN ROY, JI SUN MOON, SUNG HEUM PARK, ALAN HEEGER, University of California - Santa Barbara — The synthesis and testing of new photoactive polymers is steadily improving the light conversion efficiencies of organic bulk heterojunction solar cells. Understanding the physical interactions between the polymer donor material and the electron acceptor is critical in controlling and optimizing the morphology of the blend. While interactions between the donor and acceptor in the blend determine the scale and stability of lateral phase separation, interactions between the constituents of the blend and the neighboring device layers are equally important. In this work, we demonstrate that bulk heterojunction constituents in a polymer solar cell tend to vertically phase-separate due to differences in surface energies leading to surface-directed spinodal decomposition and / or a wetting layer. Using a combination of cross-sectional transmission electron microscopy (TEM), variable angle spectrophotometric ellipsometry (VASE), and a contact angle study, we probe the vertical phase separation in poly[3-hexylthiophene] (P3HT:PCBM) and poly[N,N′-heptadecanoyl-7,7-carbazole-alt-5,5-(4′,7′-di-2-thienyl-2,1,3-benzothiadiazole)] : [6,6]-phenyl-C61-butyric acid methyl ester (PCDTBT:PC70BM).

12:15PM B20.00004 Investigation of the bulk heterojunction structure of organic photovoltaica using neutron reflectivity, JONATHAN KIEL, Michigan State University Department of Chemical Engineering and Materials Science, BRIAN KIRBY, National Institute of Standards and Testing Center for Neutron Research, MICHAEL MACKAY, University of Delaware Materials Science and Engineering — Organic photovoltaics have received much attention recently due to their promise of affordable and flexible solar power. A major component of these devices is the bulk heterojunction: an interconnected mixture of an electron donor, a highly conjugated polymer, and an electron acceptor, generally a fullerenic derivative. We have performed neutron reflectivity experiments on 200 nm thick films of poly[3-hexylthiophene] and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) to investigate the structure of this bulk heterojunction. We observe a gradient of PCBM throughout the film that depends on processing conditions, ratio of polymer to PCBM and choice of solvent. These results are compared to working devices to show which bulk heterojunction structures are more suitable to highly efficient solar cells.
doped organic semiconductor photovoltaics, WENTING LI, CHRISTOPHER MURRAY, Department of Chemistry, CHERIE KANG, Department of Electrical and Systems Engineering, University of Pennsylvania — Hybrid solar cells based on nanocomposite organic semiconductors and IR sensitive PbSe nanocrystals (NCS) and nanowires (NWs) are fabricated and serve as a model system to test in PV devices. Wet chemical routes are used to synthesize PbSe NCS tunable in size, from 6 to 12nm in diameter, and in shape by tailoring the reaction temperature and selection of surfactants. PbSe NWs are also synthesized through oriented attachment in solution of NC building blocks to form straight, zigzag, helical, and branched NWs. We integrate PbSe NCS and NWs with the organic semiconductors P3HT and pentacene. We are able to fabricate organic-inorganic bulk heterojunctions with pentacene using a solution-processable precursor that is thermally converted to pentacene. We investigate the role of the organic semiconductor pentacene in the solar cell, both as a conductivity booster and as a more stable alternative to P3HT. We find that ligand exchange significantly increases photocurrent by replacing oleic acid ligands used in NC synthesis with shorter pyridine or octylamine ligands. We also report that tailoring the size and shape of the NCS and controlling the deposition and annealing conditions of the nanocomposites enhances the solar cell performance.

12:39PM B20.00006 Transient photovoltaic behavior of air-stable inverted organic solar cells with solution-processed electron transport layer and high work function top electrode, CHANG SU KIM, YUEH-LIN (LYNN) LOO, CHEMICAL ENGINEERING, PRINCETON UNIVERSITY TEAM — In this study, we made air-stable inverted organic solar cells comprising sol-gel derived TiOx as the electron transport layer and Au as the high work function top electrode. The highly transparent TiOx layer, placed between the ITO cathode and the active layer, smooths out ITO and provides better alignment of energy levels for electron transport. The conductivity of TiOx is known to increase with increasing exposure time to light as the excited electrons fill up shallow traps during illumination. The short circuit current of our inverted solar cells thus increases from 1.41mA/cm2 to 8.13mA/cm2 under continuous illumination for 10 minutes. In addition, when our inverted solar cells are stored in air for extended periods of time, the open circuit voltage increases due to oxygen doping of poly(3-hexylthiophene). Exposure to air for 2 days, for example, increases the open circuit voltage from -0.38V to -0.53V.

12:51PM B20.00007 Controlling Photovoltaic Loss: Recombination of Dissociated Electrons and Holes in Organic Solar Cells, ZHIHUA XU, HUIDONG ZANG, BIN HU — This presentation reports the studies of charge-transfer complex states formed from the recombination of dissociated electrons and holes at the donor-acceptor interfaces in bulk-heterojunction organic solar cells based on magnetic field effects of photocurrent. Our studies indicate that the formation of charge-transfer complex states is determined by the competition between Coulombic attraction and electrical drifting. Externally, applying electric field can clearly decrease the density of charge-transfer complex states through electrical drifting. Internally, morphology can change the competition between Coulombic attraction and electric drifting through dielectric fields and charge mobilities, and consequently affects the formation of charge-transfer complex states. As a result, changing internal dielectric fields and charge mobilities through internal Coulomb interaction and electrical drifting presents as two mechanisms to control the formation of charge-transfer complex states towards the improvement of photovoltaic efficiencies in organic bulk-heterojunction solar cells.

1:03PM B20.00008 Photo-induced improvement of Bulk Heterojunction Polymeric Solar Cells, KAMIL MIELCZAREK, ALEXANDER COOK, ANVAR ZAKHIDOV, University of Texas at Dallas, NANOTECH INSTITUTE TEAM — The effectiveness of BHJ polymeric cells depends highly on the formation of continuous three dimensional interconnecting networks of electron donor (typically RR P3HT) and acceptor (typically PCBM) materials. This process is controlled by post-processing heat treatment to induce phase separation of the materials. We demonstrate in this presentation, that in-situ photo-excitation of the BHJ structure during the annealing process controls both the maximal photocurrent and filling factor of the BHJ solar cells. We have found that variations in intensity and spectral composition of the photo excitation affect the resulting morphology of BHJ. The increased diffusivity of constituents and photo-modulation of the carrier recombination upon annealing is discussed as one of the causes of the observed morphology improvement.

1:15PM B20.00009 High-Vacuum Annealing of Polythiophene:Methanofullerene Bulk Heterojunction Solar Cells, JENNIFER SEGUI, State University of New York - Stony Brook, IOANA GEARBA, Brookhaven National Laboratory, MICHAEL RAFAEL, United States Department of Energy, CHARLES LE, United States Department of Energy — Solar cell device architectures incorporating photoactive layers of immiscible blends of organic semiconductors achieve improved photovoltaic power conversion efficiency compared to planar device geometries. We have fabricated bulk heterojunction solar cells with active layer blends of poly-3 hexylthiophene (P3HT) and the fullerene derivative, [6,6] phenyl C61-butyric acid methyl ester (PCBM). Spin casting the blend from a chlorobenzene solution forms nanometer-scale domains of electron donor and acceptor phases in the device active layer. We solve the process active layers in ambient atmospheric conditions prior to aluminum contact evaporation resulting in inevitable oxygen adsorption in the P3HT layer and interfaces. We have investigated several device post-fabrication thermal treatments for driving oxygen from the device active layer, including different temperatures, times, and vacuum pressures. We evaluate the efficacy of this technique in improving Al contact quality, film morphology, solar cell efficiency, and reproducibility via analysis of device current-voltage characteristics and tapping mode atomic force microscopy.

1:27PM B20.00010 Optimizing Ionic Electrolytes for Dye-Sensitized Solar Cells, XIAOJUAN FAN, SARAH HALL, State University of New York - Stony Brook, DEBRA SHEPHERD, Department of Chemistry, SUNY - Stony Brook, I.R. GEARBA, C.-Y. NAM, R. PINDAK, C.T. BLACK — Organic photovoltaic device power conversion efficiencies are limited in part by low charge mobility within the constituent active layer. For example, the p-type polythiophene polymers used in the highest efficiency organic photovoltaic devices have transverse hole mobilities of only $10^{-4}$-$10^{-5}$ cm$^2$/V-s, despite showing significantly higher values (~0.1 cm$^2$/V-s) in a lateral FET geometry. This mobility anisotropy is caused by poor overlap of π−π orbitals in the transverse direction, which impedes charge hopping between polymer chains. We have increased the transverse hole conductivity by as much as three times by incorporating the radical initiator di-tert-butyl peroxide into polythiophene thin films. The initiator promotes thermal crosslinking upon annealing at 170C. Crosslinked photovoltaic films maintain a similar absorption spectrum to the uncrosslinked material. Grazing incidence X-ray measurements correlate film structural changes to the measured electronic properties, and reveal two possible mechanisms for increased π−π overlap in crosslinked films. We have increased the power conversion efficiency of planar photovoltaic devices composed of p-type polythiophene and n-type C60 by about three times (from 0.9% to 2.7%) by crosslinking the polythiophene material. Moreover, crosslinked polythiophene films are rendered insoluble and thus amenable to the further material processing.
1:51PM B20.00012 Modeling photocurrent transients in organic solar cells. INCHAN HWANG, NEIL GREENHAM, Cavendish Laboratory, Department of Physics, University of Cambridge, J. J. Thomson Ave., Cambridge CB3 0HE, United Kingdom — We investigate the transient photocurrents of organic photovoltaic devices by numerical modeling of the drift-diffusion equations. Understanding charge transport in organic solar cells is one of the major interesting issues relevant to improving performance of organic devices. We demonstrate the simulation of the transient photocurrents in a response to a sharp turn-on illumination. Our results show the transient time in photocurrents is determined not only by free charge transport, but also by geminate charge pair dynamics. The dissociation probability of geminate charge pairs is a key parameter in determining the performance of organic devices, controlling the efficiency at low intensity, and also governing the fate of charge pairs formed by bimolecular recombination at high intensity. Bimolecular recombination appears to shorten the typical distance traveled by free charges from where they are generated to the electrode, leading to a reduced turn-on time at high intensity.

2:03PM B20.00013 Conjugated Polymer Organic Solar Cells made using Low Bandgap Vinylene-linked Benzothiadiazole-thiophene, N. C. HESTON, Univ. of Florida, J. MEI, S. VASILYEVA, J. R. REYNOLDS, Univ. of Florida — With over 70% of the solar photon flux occurring at wavelengths beyond 700 nm, the broad absorption spectra of low bandgap conjugated polymers offers an additional path towards improving organic photovoltaic efficiencies. Here, we report on polymer solar cells fabricated using a vinylene-linked benzothiadiazole-thiophene polymer and [6,6]-phenyl-C_{61}butyric acid methyl ester (PCBM) blends. We have fabricated cells with various blend film polymer to PCBM ratios as well as film thicknesses and architectures. The performance of these cells was investigated using both AM 1.5 and incident photon to current efficiency measurements. Surface morphologies were characterized using atomic force microscopy. A strong correlation was observed between the percentage of polymer in the blend and the resulting film morphology. We observed photon-generated currents at wavelengths greater than 800nm, though we have not yet obtained high overall power conversion efficiencies.

Monday, March 16, 2009 11:15AM - 2:15PM — Session B21 DMP: Focus Session: Dopants and Defects in Semiconductors

11:15AM B21.00001 Hydrogen multicenter bond in oxide and nitride semiconductors1, ANDERSON JANOTTI, University of California - Santa Barbara — Hydrogen is a very reactive atom, occurring in virtually all organic and in many inorganic compounds. It can form a purely covalent bond, in which two hydrogen atoms share a pair of electrons in a two-electron two-center bond, as well as polar covalent bonds, such as in an H_{2}O molecule. In solids, hydrogen is usually considered as an interstitial impurity. In elemental semiconductors, such as silicon, hydrogen forms a three-center bond when located at the bond center. In compound semiconductors, hydrogen bonds to the anionic species in p-type material, and to the cationic species in n-type. Thus far, hydrogen in solids has been found to form chemical bonds with one, two, or at most three other atoms. Higher coordination numbers are exceedingly rare and have been reported only for clusters. In this talk we will show that hydrogen is capable of forming multicenter bonds in solids, occupying substitutional sites. As examples, we discuss substitutional hydrogen impurities in oxides (ZnO, MgO, SnO_{2}, TiO_{2}) [1,2] and nitrides (InN, AIN, GaN) [3]. Based on first-principles calculations we show that hydrogen replaces oxygen (nitrogen) and forms genuine chemical bonds with multiple metal atoms, in truly multicoordinated configurations. These multicenter bonds are surprisingly strong despite the large hydrogen-metal distances when compared to typical values in hydrogen two-center bonds. Hydrogen in the multicenter bond configuration is a shallow donor in a number of materials. In conducting oxides, it provides a consistent explanation for the observed dependence of electrical conductivity on oxygen partial pressure, thus resolving a long-standing controversy on the role of point defects in unintentional n-type conductivity [1,2].


1In collaboration with C. G. Van de Walle, this work was supported by the NSF MRSEC Program under Grant No. DMR05-20415 and by the UCSB Solid State Lighting and Energy Center.

11:51AM B21.00002 Hydrogen in anion vacancies of semiconductors1, MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — Hydrogen typically terminates the dangling bonds around vacancies in semiconductors, thereby, partially or completely passivating the vacancies. However, it has been shown recently that hydrogen in anion vacancies of many semiconductors, such as ZnO, MgO, InN, SnO_{2}, and GaN, takes multi-coordinated structures and acts as shallow donors, providing n-type conductivity to the materials. We study the hydrogen in the anion vacancies of a series of II-VI and III-V semiconductors using density functional calculations. The results on these materials show that, in the anion vacancies of polar II-VI semiconductors, the hydrogen is usually anionic and is coordinated with more than one cation atoms as a result of the relatively high ionization of the host material. The hydrogen coordination number depends on the host anion size. On the other hand, in more covalent semiconductors such as some III-V semiconductors, the single cation-H bonding configuration may become most stable. In the anion vacancies of ZnX and CdX where X represents anions, hydrogen is typically amphoteric except for oxides, in which the small anion size prohibits the formation of the cation-cation bond that is required for the acceptor configuration.

1This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22.

12:03PM B21.00003 Defect Creation and Annihilation in GaN and ZnO1, CHRIS VAN DE WALE, ANDERSON JANOTTI, University of California, Santa Barbara — ZnO is an extremely attractive material for a number of optoelectronic and electronic applications. Among its advantages is its radiation hardness, which is even greater than that of GaN. Based on our comprehensive investigations of intrinsic point defects [1,2], we have developed a model for defect creation and annihilation during and after irradiation. The calculations, based on pseudopotential-density-functional theory combined with LDA+U [2] produce formation energies, stability of charge states as a function of Fermi level, and migration barriers for each of the point defects. Migration barriers allow us to determine annealing temperatures at which we predict various defects to be mobile. In ZnO, the key factors responsible for radiation hardness are the low migration barriers of point defects and the charge-state matching of dominant defect pairs. Quantitative arguments for both ZnO and GaN will be presented, and the results compared with experimental observations. The insights provided by our modeling can be fruitfully applied to understand irradiation effects in semiconductors and insulators in general. [1] S. Limpijumnong and C. G. Van de Walle, Phys. Rev. B 69, 035207 (2004). [2] A. Janotti and C. G. Van de Walle, Phys. Rev. B 76, 165202 (2007).

1Work supported by the NSF MRSEC Program under award No. DMR05-20415.
12:15PM B21.00004 Asymmetric hole localization and multiple hole binding of acceptors in ZnO\(^1\). STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory — Holes bound at cation-site acceptors in oxides, such as Li\(_{2}\), or the Zn vacancy in ZnO tend to be localized on a single oxygen neighbor rather than to be delocalized over symmetrically equivalent sites. As a consequence of this localization, the acceptor level lies deep in the gap, typically \(\sim 1\) eV above the VBM. In contrast, conventional local density calculations do not show this symmetry breaking, and predict the acceptor level much too shallow. This failure of approximate functionals has been attributed to the residual self-interaction, which underestimates the energy splitting between occupied and unoccupied states. We identify a criterion for the cancellation of the self-interaction in terms of a generalized potential \(\hat{V} = \hat{V}\left(r_2, r_3, \ldots, r_n\right)\) using this criterion to define a self-interaction correction (SIC) potential that does not rely on empirical parameters. After the SIC, the unoccupied hole states are correctly placed in energy with respect to the spectrum of the occupied host states. We use this method to predict the acceptor levels of cation-site acceptors and the Zn vacancy in ZnO, and of acceptors in In\(_2\)O\(_3\) and SnO\(_2\). We find that these acceptors have too deep levels to cause \(p\)-type conductivity, and we further predict that nominal single acceptors can generally bind multiple holes (up to 3).

\(^1\)Funded by DOE-EERE under contract DE-AC36-08GO28308.

12:27PM B21.00005 ABSTRACT WITHDRAWN

12:39PM B21.00006 ABSTRACT WITHDRAWN

12:51PM B21.00007 Unusual uniaxial stress results on the stretch mode of OH related defects in ZnO. KEVIN MARTIN, University of Pittsburgh at Johnstown, Johnstown PA, W. BEALL FOWLER, Lehigh University, Bethlehem PA — Some uniaxial stress studies of the frequency dependence of O-H related defects in ZnO have produced surprising results\(^1\)-\(^2\). For example, the Li:OH defect in ZnO (H\(^{1+}\)) is oriented along the c-axis, yet the OH stretch mode decreases in frequency when stress is applied along the c direction and increases when stress is perpendicular to the c-direction. Another example is the Cu:OH defect, in which the OH is aligned along one of the three non-c tetrahedral directions. Stress along the c-direction produces a strongly non-linear increase in frequency. These examples and others indicate something unusual is happening in these systems. One possibility is that the piezoelectric effect in ZnO is responsible for the "backward" behavior of the frequency shift of these defects. The piezoelectric effect in ZnO is caused by the lack of cancellation between the "clamped-ion" term (i.e., electronic contribution) and the term related to the change in the u parameter ("internal strain"). With the latter dominating, when c stress is applied, the value of u increases, thus the two interpenetrating hexagonal lattices (one for Zn, the other for O) increase their overlap. We will attempt to explain the experimental results within this framework. \(^1\)Lavrov and Weber, Phys. Rev. B, 73, 035208 (2006), and \(^2\)Phys. Stat. Sol. (b) 243, 2657 (2006) \(^3\)Corso, et al Phys. Rev B. 50, 10715 (1994)

1:03PM B21.00008 Theoretical study of Si in ZnO\(^1\). JOHN LYONS, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Recently, the presence of silicon in relatively high concentrations has been detected in samples of ZnO\(^1\). The properties of this impurity have not yet been investigated. Here we present a first-principles study of the electronic and structural properties of Si in zinc-blende ZnO using density functional calculations with LDA, GGA, and hybrid functionals. Our calculations show that substitutional Si on a Zn site is lower in energy than either Si on an oxygen site or a Si interstitial. The calculations consistently predict Si to be a shallow donor in ZnO, with the \(2^+\) state being mostly stable across the band gap. The formation energy of substitutional Si is relatively low, supporting experimental evidence which shows a concentration of \(10^{17}\) cm\(^{-3}\) Si in ZnO samples. The properties of Ge in ZnO are also studied for comparison and show behavior similar to that of Si. \(^1\)M.D. McCluskey and S.J. Jokela, Physica B 401-402, 355 (2007).

\(^1\)Work supported by the NSF MRSEC Program under Grant No. DMR05-20415 and by the UCSB Solid State Lighting and Energy Center.

1:15PM B21.00009 Photoinduced EPR study of electron traps in TiO\(_2\) crystals: Oxygen vacancies and Ti\(^{3+}\) ions. SHAN YANG, ADAM BRANT, LARRY HALLIBURTON, Physics Department, West Virginia University — Electron paramagnetic resonance (EPR) provides a sensitive method to monitor native defects in wide-band-gap semiconductors. In-situ illumination with laser light at low temperature (photoinduced EPR) forms paramagnetic defects in fully oxidized bulk TiO\(_2\) crystals. Illumination with 442 nm laser light at 30 K and below produces four electronlike centers and one hololex center. Three of the electronlike centers have S = \(1/2\) and are assigned, respectively, to a substitutional Ti\(^{3+}\) ion in the otherwise perfect lattice, a substitutional Ti\(^{3+}\) ion adjacent to a Si\(^{4+}\) ion, and a substitutional Ti\(^{3+}\) ion adjacent to an oxygen vacancy. The fourth electronlike center has S = 1 and is assigned to two Ti\(^{3+}\) ions adjacent to one oxygen vacancy. The hololex center has S = \(1/2\) and consists of a hole shared equally by two adjacent oxygen ions in the otherwise perfect lattice. Spin-Hamiltonian parameters, obtained from complete sets of angular dependence data, are presented for each of the centers. This work was supported by NSF Grant No. DMR-0804352.

1:27PM B21.00010 The nature of Group-V acceptor impurities in SnO\(_2\)^{1}. JOEL VARLEY, Department of Physics, University of California at Santa Barbara, ANDERSON JANOTTI, CHRIS VAN DE WALLE, Materials Department, University of California at Santa Barbara — Group-V elements have long been considered leading candidates for achieving p-type doping in semiconducting oxides. Using first-principles calculations, we investigate the feasibility of achieving ambipolar doping in SnO\(_2\) using the Group-V elements N, P, and As. We address the electronic structure of these impurities by performing systematic density functional calculations using hybrid functionals. This approach overcomes the band-gap problems inherent in calculations using the local density approximation or generalized gradient approximation, thus allowing us to accurately determine energies of defect levels. We discuss the stability of the isolated impurities both as substitutional and interstitial defects, based on calculated formation and migration energies. We also investigate their possible passivation by hydrogen and examine binding energies and activation energies of hydrogen-acceptor complexes. We conclude that the Group-V elements are deep acceptors that will not enable p-type doping of SnO\(_2\).

\(^1\)This work was supported by the NSF MRSEC Program under award No. DMR05-20415.

1:39PM B21.00011 Manipulation of Single Oxygen Vacancies on TiO\(_2\)(110). DANDA ACHARYA, PETER SUTTER, Brookhaven National Laboratory — Oxygen vacancies are among the primary chemically active defects on the surface of reducible transition metal oxides, playing a key role in surface chemistry, catalysis, and photocatalysis. We report the controlled manipulation of individual O-vacancies on reduced TiO\(_2\)(110)-1\_1 using a low temperature scanning tunneling microscope. Localized voltage pulses trigger the hopping of single vacancies along a bridging oxygen (O\(_{\text{av}}\)) row. We discuss the microscopic manipulation mechanism and demonstrate atomic-scale control by constructing linear and more complex arrangements of vacancies. Single defect manipulation is used to probe the interaction of closely spaced vacancies, and to establish the possibility of forming highly reactive double and a triple O-vacancy clusters. Detailed experimental and theoretical analysis reveals that bridge-bonded O-vacancy pairs are stable and have lower energy than pairs of vacancies separated by two or more lattice spacings. The existence of stable vacancy pairs with exposed low-coordinated Ti atoms has implications on the reactivity of TiO\(_2\)(110) and of similar metal oxide surfaces.
1:51PM B21.00012 Coordination Defects and Nanoclusters of TiO$_2$. KEN PARK, Baylor University. VINCENT MEUNIER, MINGHU PAN, Oak Ridge National Laboratory, NAN-HSIN YU, Baylor University, WARD PLUMMER, Louisiana State University — Titanium oxide is one of the most investigated photocatalytic systems. It is capable of converting toxic organic and inorganic materials to benign products, as well as turning solar energy into a chemical one. Many believe that the catalytic activation involves charge transfer localized at surface defects with lower stoichiometry and/or coordination. In this study, scanning tunneling microscopy (STM) and density functional theory (DFT) are used to gain insight into such defects on TiO$_2$(110). STM reveals defects ranging from a few Angstroms to a few nanometers in size, but all of a uniform height of 3 Å. These topographically distinct defects are determined as fully stoichiometric nanoclusters by DFT. Despite the full stoichiometry, they possess undercoordinated atomic sites including 3- and 4-coordinated Ti and 1-coordinated O atoms. Their electronic and chemical properties will be discussed.

1Supported in part by the Office of Basic Energy Sciences, U. S. DOE.

2:03PM B21.00013 Kinetic Monte Carlo study for the thermal stability of hydrogen in ZnO. JUNHYEOK BANG, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701 — Zinc oxide (ZnO) has attracted much attention due to a variety of applications to transparent optoelectronic devices. It is known that undoped ZnO exhibits n-type conductivity. Hydrogen, which is unintentionally incorporated, is considered as a promising candidate for shallow donors in ZnO. However, it is still difficult to explain n-type conductivity in annealed ZnO due to the low thermal stability of H. Here we study the diffusion of H in ZnO using first-principles calculations and then perform kinetic Monte Carlo (kMC) simulations for the thermal stability of H. The migration energy of a substitutional H is much higher than that for an interstitial H. Using as input the energy barriers for H diffusion, kMC simulations show that interstitial and substitutional H atoms diffuse out at different annealing temperatures around 125 and 475 °C, respectively, in good agreement with experiments. When H atoms are injected from air into ZnO, we find that they are likely to be trapped at O-vacancy sites, leading to the n-type conductivity in annealed samples.

Monday, March 16, 2009 11:15AM - 2:03PM –
Session B22 GMAG DMP FIAP: Focus Session: Theory of Spin-based Semiconductor Devices

11:15AM B22.00001 Role of motive forces for the spin torque transfer for nano-structures. STEWART BARNES, Physics Department, University of Miami — Despite an announced imminent commercial realization of spin transfer random access memory (SPRAM) the current theory evolved from that of Slonczewski [1,2] does not conserve energy. Barnes and Maekawa [3] have shown, in order correct this defect, forces which originate from the spin rather than the charge of an electron must be accounted for, this leading to the concept of spin-motive-forces (smf) which must appear in Faraday’s law and which significantly modifies the theory for spin-valves and domain wall devices [4]. A multi-channel theory in which these smf’s redirect the spin currents will be described. In nano-structures it is now well known that the Kondo effect is reflected by conductance peaks. In essence, the spin degrees of freedom are used to enhance conduction. In a system with nano-magnets and a Coulomb blockade [5] the similar spin channels which these smf’s redirect the spin currents will be described. In nano-structures it is now well known that the Kondo effect is reflected by conductance peaks. In essence, the spin degrees of freedom are used to enhance conduction. In a system with nano-magnets and a Coulomb blockade [5] the similar spin channels which these smf’s redirect the spin currents will be described. In nano-structures it is now well known that the Kondo effect is reflected by conductance peaks.


1Supported in part by the EPSRC, UK.

11:51AM B22.00002 Revisiting the “Spin-Transistor”. ABU NASER ZAINUDDIN, LUTFE SIDDIQUI, SUPRIYO DATTA, Purdue University — A “spin-transistor” in principle requires efficient injection (source), efficient detection (drain) and electrical manipulation (gate). For sometime now, electrical manipulation based on the Rashba effect has been well established and in recent years there has been significant progress in the design of injectors and detectors. Lateral spin-valve structures showing ~50% spin-polarization has been reported. In view of these advances it seems appropriate to evaluate various “spin-transistor” concepts. With this in mind, we have developed non-equilibrium Green’s function (NEGF) based model and benchmarked against existing experiments.

12:03PM B22.00003 Dynamical magnetoelectric feedback effects in magnetic resonant tunneling structures. CHRISTIAN ERTLER, JAROSLAV FABIAN, Institute for Theoretical Physics, University of Regensburg — Heterostructures made of stacked layers of both magnetic and nonmagnetic semiconductors provide a lot of opportunities for controlling and tuning their spin-dependent transport properties. For instance, highly efficient spin valves, spin switching and spin filtering devices have been demonstrated by using magnetic resonant tunneling structures [1]. Here, we show that in a resonant tunneling double barrier structure, which comprises a ferromagnetic quantum well made of a dilute magnetic semiconductor material, interesting dynamical effects can occur [2]. In such systems the transport and magnetic properties become strongly coupled, since the ferromagnetic order in the quantum well is determined by the itinerant carriers. Both the Coulomb interaction of the particles well as the magnetic exchange field give rise to strong feedback effects on the tunneling current. Interestingly, for a broad voltage range self-sustained high-frequency oscillating currents associated with an oscillating well magnetization appear. The requirements for the occurrence of these dc-driven magnetoelectric oscillations are investigated and possible device setups, which should allow for an experimental observation, are discussed. [1] J. Fabian, A. Matos-Abiague, C. Ertler, P. Stano and I. Zutic, Acta Phys. Slov. 57, 565 (2007). [2] C. Ertler and J. Fabian, Phys. Rev. Lett. 101, 077202 (2008).

1This work has been supported by the Deutsche Forschungsgemeinschaft SFB 689.
12:15PM B22.00004 Theory of Semiconductor Spin Lasers, CHRISTIAN GOTHGEN, SUNY Buffalo, RAFAL OSZALDOWSKI, SUNY Buffalo and N. Copernicus University, Torun, Poland, IGOR ZUTIC, SUNY Buffalo — Semiconductor lasers with spin-polarized carriers’ injection have important advantages as compared to the conventional lasers in which the carriers are unpolarized. While such spin lasers have been successfully realized and shown to provide spin-polarization modulation and threshold current reduction [1-4], there remain important theoretical challenges in understanding their operation. We demonstrate that the maximum threshold reduction is larger than previously thought possible and, surprisingly, can be enhanced by ultrafast spin relaxation of holes [5]. By combining our analytical model [5] and numerical studies of spin lasers we explore the effects of quantum confinement in the gain region and identify different modes of operation. We thank A. Petrou for valuable discussions. This work is supported by US ONR and NSF-ECCS CARRER.


12:27PM B22.00005 Design Guidelines for Spin-Polarized Lasers, MICHAEL HOLUB, IGOR VURGAFTMAN, JERRY MEYER, BEREND JANONKER, Naval Research Laboratory — Semiconductor lasers driven by a spin-polarized current are expected to provide a threshold current reduction and optical polarization control. The design of spin-polarized lasers is critical to the realization of these effects. Thus, we have investigated the effect of electron spin injection on semiconductor laser performance using a spin-dependent rate equation model. The magnitude of the threshold reduction is shown to depend on intrinsic properties of the active region and laser cavity, and can approach a factor of 3.5 for fully spin-polarized electrons. The threshold reduction is found to be strongest in lasers with undoped active regions, recombination strongly dominated by Auger processes, and low threshold gain. Introduction of a ferromagnetic electrode in the vicinity of the active region for efficient spin injection generally results in higher internal loss and a requirement for greater material gain, which raises the laser’s baseline threshold as well as lessens the projected threshold reduction. The placement of a ferromagnetic contact on spin-polarized laser performance will be discussed.


12:39PM B22.00006 Spin-orbit coupling effects in Fe/GaAs heterostructures: First principles calculations, MARTIN GMITRA, ALEX MATOS-ABIAIGUE, University of Regensburg, Germany, CLAUDIA AMBROSCH-DRAXL, University of Leoben, Austria, JAROSLAV FABIAN, University of Regensburg, Germany — The tunneling anisotropic magnetoresistance (TAMR) effect in semiconductor heterostructures containing a single ferromagnetic layer is potentially useful for spintronics devices. Important, TAMR has recently been observed in a metallic system, namely, in Fe/GaAs/Au junctions. Surprisingly, while all the bulk components of the system are cubic, the observed anisotropy is twofold, of the C2v class. This suggests that rather than coming from the bulk anisotropy of the density of states, the effect arises from the interface that indeed has a reduced symmetry. A phenomenological model reflecting this symmetry in the form of the Bychkov-Rashba and the Dresselhaus spin-orbit coupling was proposed, giving a quantitative fit to the experiment. Here we report on comprehensive first principle calculations of the spin-orbit effects stemming from the interface anisotropy, providing support to the phenomenological theory. In particular, we have performed FPLAPW density functional calculations of an Fe/GaAs slab to extract quantitative information about the proposed model that are Bychkov-Rashba and Dresselhaus parameters.

1Financial support via SFB 689 is gratefully acknowledged.

12:51PM B22.00007 Magnetic phase transitions driven by non-equilibrium spins and their potential applications to magnetic cooling, LUTFE SIDDIQUI, ABU NASER ZAINUDDIN, SUPRIYO DATTA, School of Electrical and Computer Engineering, Purdue University — It is well-known that the Curie temperature in diluted magnetic semiconductors (DMS) like GaMnAs can be controlled by changing the equilibrium density of holes in the material. In this letter we predict, that even with a constant hole density, large changes in the magnetization can be obtained with a relatively small imbalance in the spin population. In particular, the structure under consideration consists of a three ferromagnetic dielectric layers, which are coupled through monolayer graphene placed in interface between two magnetic dielectric layers. We find that by combining the electrical effect on the exchange bias field and a giant magneto-resistance effect of the graphene/ferromagnet hybrid structures, a non-volatile magnetic field can be obtained instead of an external magnetic field with high energy consumption. In particular, the structure under consideration consists of three ferromagnetic dielectric layers, which are coupled through monolayer and bilayer graphene films. Interplay of two graphene layers can mediate the exchange bias fields applied to different sides of the free ferromagnets resulting in programmable logic operations.

1This work was supported in part by the DARPA and the FENA

1:03PM B22.00008 Magnetic memory and logic based on spin effects in graphene, JOHN ZAVADA, YURIY SEMENOV, KI WOOK KIM, NCSU — We report on a novel approach to the problem of low-power-consuming non-volatile magnetic random access memory (MRAM) and logic design that is based on the unique properties of the graphene placed in interface between two magnetic dielectric layers. We find that by combining the electrical effect on the exchange bias field and a giant magneto-resistance effect of the graphene/ferromagnet hybrid structures, a non-volatile magnetic field can be obtained instead of an external magnetic field with high energy consumption. In particular, the structure under consideration consists of a three ferromagnetic dielectric layers, which are coupled through monolayer and bilayer graphene films. Interplay of two graphene layers can mediate the exchange bias fields applied to different sides of the free ferromagnets resulting in programmable logic operations.

1:15PM B22.00009 Metal-insulator transition in a quantum wire with alternating Rashba interaction, HENRIK JOHANNESSON, University of Gothenburg, Sweden, GEORGE I. JAPARIDZE, Andronikashvii Institute of Physics, Tbilisi, Georgia, ALVARO FERRAZ, ICCMP, Brazil — We propose and analyze a device scheme by which an electrical current can be controlled via a gate-operated spin-orbit interaction. The device consists of a quasi-one-dimensional (1D) ballistic channel in a gated semiconductor heterostructure, contacted to a source and a drain and with the gates producing an alternating Rashba spin-orbit interaction. When the period of the Rashba modulation becomes commensurate with the 1D electron density, the spin-orbit interaction opens a charge gap, leading to a suppression of the current. Using bosonization and a perturbative RG approach we explore how electron-electron interactions influence the effect.

1:27PM B22.00010 Gate control of single-electron spins through Berry Phase in a realistic asymmetric confining potentials in III-V semiconductor Quantum Dots, SANJAY PRABHAKAR, JAMES RAYNOLDS, Ublbany Nanoscience — Among recent proposals for next-generation, non-charge-based logic is the notion that a single electron can be trapped and its spin can be manipulated through the application of gate voltages (Rev. Mod. Phys.79, 1217 (2007)). In this talk we present numerical simulations of Berry Phase of electron spins in single electron devices for realistic asymmetric confining potentials in support of experimental work at the University at Albany, State University of New York at the practical development of post-CMOS concepts and devices. We solve the Schrodinger equation including spin-orbit using a special numerical algorithm. The design of a quantum dot will be presented. The Berry Phase for electrons in a dot is calculated for both 0 and finite gate bias. The Berry Phase is calculated for a dot with an electrostatically defined quantum dots including the Rashba and Dresselhaus spin-orbit interactions computed numerically from realistic asymmetric confining potentials. The new simulation results open the possibility of spin manipulation through the gate induced Berry phase. This work is supported through funding from the DARPA/NRI INDEX center.

1:51PM  B22.00012  impurity-impurity interaction in graphene nanoribbons, JIAN-MING TANG, University of New Hampshire — The high mobility and small spin-orbit interaction makes graphene a promising candidate material for building spin-based quantum devices. Embedded magnetic dopants or magnetized defects may act as single spin qubits in these devices. The long decay length for the impurity levels near the Dirac point suggest that the double exchange interaction can compete with the RKKY exchange interaction. The impurity level splitting for two impurities in bulk and in nanoribbons are studied using a tight-binding approach. In the case of nanoribbons, the modification to the interaction due to the presence of edge states will be discussed.


11:15AM  B23.00001  Optimized basis-set representation for electronic-structure methods: Better Energetics1, AFTAB ALAM, DUANE JOHNSON, University of Illinois at Urbana Champaign — We derive an analytic expression for an optimal, and rapidly computed, representation for site-centered basis-set expansion (e.g., spherical harmonic). An optimal site-dependent radius are determined from the local saddle-point derived in terms of overlapping atomic charge densities, typically already used for Löwden construction of the starting potentials. These “saddle-point adjusted” sphere radii separate the “spherical” density and potential around an atom from the symmetry-induced, “non-spherical” part in the interstitial, and more properly accounts for charge and size of atoms. These radii also properly determine the weighted Voronoi cells (i.e., power diagram or “saddle-point adjusted” sphere radii separate the “spherical” density and potential around an atom from the symmetry-induced, “non-spherical” part in the interstitial, and more properly accounts for charge and size of atoms). We implement these ideas in a general Korringa-Kohn-Rostoker coherent potential approximation electronic-structure method, we present results using the dynamical cluster approximations (DCA) to obtain the temperature-dependent SRO in disordered alloys. We obtain the KKR-DCA SRO energetics versus local neighbor SRO parameters and minimize it at fixed temperature to predict the SRO. We show that the calculated SRO at fixed temperature compares well with experimental results, and then correlate the results to the electronic structure. We discuss how an accurate analytic estimate can be made for the SRO in most metals due to the dependence of the grand potential on SRO.

1Department of Energy under BES grants (DE-FG02-03ER4602631) and (LLNL-B573247).

11:27AM  B23.00002  Applications of the KKR-DCA: A Finite-Temperature Density Functional Theory to Predict Chemical Short-Range Order Effects in Disordered Metallic Alloys1, D.A. BIAVA, D.D. JOHNSON, University of Illinois — Short-range order (SRO) is ubiquitous in metallic alloys, affecting changes in their electronic, thermodynamic, mechanical, magnetic, and structural properties. For example, SRO is responsible for the yield-strength anomalies observed in Cu-Al at high temperatures, i.e., the materials is more resistant to dislocation motion at high temperature than it is at room temperature. Within the Korringa-Kohn-Rostorker (KKR) electronic-structure method, we present results using the dynamical cluster approximations (DCA) to obtain the temperature-dependent SRO in disordered alloys. We obtain the KKR-DCA SRO energetics versus local neighbor SRO parameters and minimize it at fixed temperature to predict the SRO. We show that the calculated SRO at fixed temperature compares well with experimental results, and then correlate the results to the electronic structure. We discuss how an accurate analytic estimate can be made for the SRO in most metals due to the dependence of the grand potential on SRO.

1Work supported by the National Science Foundation under grant DMR-0705089.

11:39AM  B23.00003  Electronic and Magnetic properties of NbFe2: An itinerant magnet near a quantum critical point1, ALASKA SUBEDI, DAVID J. SINGH, Materials Science and Technology Division, ORNL — NMR studies show that pure C14 Laves phase NbFe2 is a weak antiferromagnet below 13K with magnetic moment per Fe of no more than 0.1μB. However, the Nb-rich samples do not show antiferromagnetism down to 1.8K, which suggests that they are close to antiferromagnetic QCP. Here we report density functional studies of the magnetic properties, band structure and Fermiology. We elucidate the nature of the ordering between the two distinct Fe sites and discuss the results in relation to the quantum criticality.

1Work supported by DOE - DMSE.

11:51AM  B23.00004  First-principles calculations of free energies of unstable phases: The case of fcc W, VIVDUOS OZOLINS, Department of Materials Science & Engineering, University of California, Los Angeles — Ab initio density-functional theory molecular dynamics simulations are used to solve the long-standing problem of calculating the free energies of harmonically unstable phases, such as fcc W. We find that fcc W is mechanically unstable with respect to long-wavelength shear at all temperatures considered (T>2500 K), while the short-wavelength phonon modes are anharmonically stabilized. The calculated fcc/bcc enthalpy and entropy differences at T=3500 K (308 meV and 0.74 kB per atom, respectively) agree well with the recent values derived from analysis of experimental data. The proposed method can be used in first-principles modeling of the thermodynamics of unstable phases and calculations of the thermodynamic driving forces for martensitic transformations in pure elements and alloys.

1The author gratefully acknowledges financial support from the National Science Foundation under grant No. DMR-0427638 and an ANL Blue Gene supercomputer award from the DOE INCITE program.
12:03PM B23.00005 Anomalies in the bulk properties of single crystalline Niobium1. RICHARD K. BOLLINGER, J. J. NEUMEIER, B. D. WHITE, Montana State University, YOKO SUZUKI, A. MICLORI, JON BETTS, National High Magnetic Field Laboratory - Los Alamos National Laboratory, H. R. Z. SANDIM, C. A. M. DOS SANTOS, Escola de Engenharia de Lorena -USP — The thermodynamic properties of single crystal Niobium are presented. Anomalies in thermal expansion, specific heat, elastic constants, and electrical resistivity are observed. The linear coefficient of thermal expansion, $\alpha$, exhibits a large, broad peak in the range 200 K $< T < 280$ K, with a nearly two-fold increase in $\alpha$. The elastic constants show anomalies over a similar temperature range, while anomalies in heat capacity and resistivity are much narrower. This is surprising since crystalline Nb is a simple system, with only one naturally occurring isotope and a body centered cubic structure. Measurements on a second single crystal and on high purity polycrystalline Nb will also be presented.

1Supported by the US DOE Office of Basic Energy Sciences (DE-FG-06ER46269). Work at LANL was conducted under the auspices of the US DOE Office of Basic Energy Sciences.

12:15PM B23.00006 Development of an Embedded-Atom Method Potential for Niobium1. MICHAEL R. FELLINGER, JOHN W. WILKINS, The Ohio State University — An embedded-atom method (EAM) potential [1,2] is developed for pure niobium as the first step in the construction of an EAM potential for titanium-niobium alloys. The potential is constructed using the force-matching method [3]: the functions comprising the potential are represented as cubic splines, and the spline knots are chosen such that the potential optimally reproduces a large database of forces, cohesive energies, and stresses computed via density functional theory. The code potfit [4] optimizes the splines using a combination of simulated annealing and conjugate gradient-like minimization algorithms. EAM results are compared to DFT and experimental results for the lattice constant, cohesive energy, single-vacancy formation energy, fcc-bcc and hcp-bcc structural energy differences, elastic constants, and phonon dispersions.


12:27PM B23.00007 Ab initio up to the melting point: Anharmonicity and vacancies in aluminum, B. GRABOWSKI, L. ISMER, T. HICKEL, J. NEUGEBAUER, Max-Planck-Institut Düsseldorf, Germany — At elevated temperatures, the heat capacity of metals strongly deviates from the harmonic prediction. This was pointed out long ago and Zn solubility in Ti from first-principles calculations showed that a dominant part can be explained by quasiharmonic excitations. However, the detailed balance of further contributions, such as explicit anharmonicity and vacancies, is not clarified yet even for simple elementary metals. Aluminum is a prototypical example. Even though intensively studied, the ambiguous experimental situation has made a classification of the mechanisms impossible. To resolve the situation, we have calculated the full volume and temperature dependent $ab$ initio free energy surface employing density-functional theory. In particular, we have included anharmonic and vacancy contributions using numerically highly efficient methods to coarse grain the configuration space. To obtain accurate vacancy energies, we have included the full spectrum of quasiharmonic excitations: quasiharmonic, electronic, and explicitly anharmonic. The results are in contradiction to common belief, nevertheless the essential physics can be captured by a simple model.

1M. Born and E. Brody, Zeitschrift für Physik 6, 132 (1921)


12:39PM B23.00008 New Generation Structural Materials: Ab initio Based Modeling of High-Entropy Alloys, G. MALCOLM STOCKS, XING-QIU CHEN, EASO P. GEORGE, CHONGLONG FU, TAKESHI EGAMI, Oak Ridge National Laboratory, Division of Materials Science and Technology, MATERIALS THEORY TEAM — There is rapidly growing interest in a new generation of structural materials called high entropy alloys. This class of alloys is multi-component (~ five elements) with approximately equiatomic ratio, and thus have high entropy of mixing by which they are distinguished from conventional alloys. It has been reported experimentally that the single bcc-based AlCoCrFeNi, single fcc-based CoCrCuFeNi and FeCrMnNiCo high-entropy alloys exhibit promising mechanical properties with potential applications. In this work, we introduce ab initio based modeling for understanding structural, magnetic, and elastic properties based on relaxation of randomly generated supercells within the framework of density functional theory. We studied component-dependent phase stabilities, electronic structures, and magnetic properties with all solutes at fixed and relaxed structures. The properties are analysed in terms of the underlying electronic structure and suggestions are made for further experimental studies to further clarify the reasons for the unusual stability of these systems. Research sponsored by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. DOE.

12:51PM B23.00009 High-throuput formalism and calculation of Ag, Au, Cd, Co, Cr, Ir, W, and Zn solubility in Ti from first-principles1. ROMAN CHEPULSKY, STEFANO CURTAROLO, Duke University — Based on statistical-thermodynamic theory of a dilute lattice gas, we developed an approach for calculation of atomic solubility in alloys. The advantage of the approach consists in taking into account all known alloy ground states rather than just pure species. It is shown that the low-solubility obey the simple Arrhenius-type dependence on temperature determined by “low-solubility formation energy.” Such quantity is defined as the derivative of the compound formation energy, determined with respect to surrounding ground states, versus composition. “Low-solubility formation energy” coincides with the usual “true” defect formation energy only in the case of a phase-separating alloy having no intermediate ground states and vacancies. We present a high-throughput formalism where the “low-solubility formation energy” can be directly obtained through first-principles calculations. The developed approach is applied to solubility of transition metals in titanium. The obtained values and tendencies are in good qualitative correspondence with experiments.

1Research was supported by ONR and NSF.

1:03PM B23.00010 Alternative alloys for catalysts and platinum jewelry? New structures in Pt-Hf and Pt-Mo, ERIN GILMARTIN, JACQUELINE CORBITT, GUS HART, Brigham Young University — The only known intermetallic structure with an 8:1 stoichiometry is that of Pt$_3$Ti. It is intriguing that an ordered phase would occur at such low concentrations of the minority atom, but this structure occurs in about a dozen binary intermetallic systems. The formation of an ordered phase in an alloy can significantly enhance the performance of the material, particularly the hardness. We have taken a broad look at possible systems where this phase forms. Using first-principles, we calculated the stability of this structure relative to experimentally known phases for more than 80 Pt/Pd binary systems. We find the Pt$_3$Ti structure is a possible ground state in more than 20 cases. Our experimental collaborators have verified our prediction in Pt-Mo and observed order-hardening in Pt-Hf. We discuss the discovery of new ground states that are likely to be verified experimentally and their impact on materials for Pt- and Pd-based catalysts and jewelry.
1:15PM B23.00011 New structures in Pd-rich ordered alloys. JACQUELINE CORBITT, ERIN GILMARTIN, GUS HART, Brigham Young University — An intriguing intermetallic structure with B1 stoichiometry was discovered in the 1950s in the Pt-Ti system. Since then a handful of other Pt/Pd/Ni binary systems have been observed to exhibit this curious structure (Pt$_x$Zr, Pd$_x$Mo, Ni$_x$Nb, etc.). This ordered structure can significantly increase the hardness of an alloy. For jewelry applications involving Pt and Pd, international hallmarking standards require that the alloys be at least 95% pure by weight. However, Pt- and Pd-rich alloys are often soft when purity is high if the minority atoms are disordered. Because the B1 structure maintains a high weight percentage of Pt/Pd, it can satisfy purity standards while increasing performance. Recent calculations and experiments suggest that the B1 structure may form in about 20 previously unsuspected Pt/Pd binary systems. Using first-principles calculations and cluster-expansion modeling, we have performed a ground state search to find the stable structures in Pt-Dnd and Pd-Cu. In collaboration with Candace Lang’s group at University of Capetown South Africa, we are working to experimentally validate the predicted ground states.

1:27PM B23.00012 Verification and refinement of the Al-Mg-Zn $\Phi$ phase crystal structure model. JEFF HOUZE, BOHUMIR JELINEK, SUNGHO KIM, SEONG-GON KIM, MARK HORSTMEYER, Mississippi State University — Density Functional Theory calculations were performed to validate the crystal structure proposed by L. Bourgeois et al. for the $\Phi$ phase of the Al-Mg-Zn system. Their model has ambiguous site occupancies for Zn and Al and definite locations for Mg. The model’s simulated electron diffraction patterns agreed very well with experimental patterns. Using DFT calculations we are able to determine optimal Zn and Al aluminum locations. We will also show that the energetically optimal structure’s element concentrations are within the experimentally observed range.

1:39PM B23.00013 An ab initio study of the crystal structure of the Tau-phase in Al-Mg-Zn alloys. LAALITHA LIYANAGE, JEFFREY HOUZE, SUNGHO KIM, MARK HORSTMEYER, SEONG-GON KIM, Center for Advanced Vehicular Systems, Mississippi State University — Existing crystal structures for the intermetallic Tau-phase in Al-Mg-Zn alloy are studied by density functional theory calculations using projector augmented wave pseudopotentials. Favorable crystal structures are identified through volume optimization and formation energy calculations. Properties such as elastic constants and bulk modulus of the crystal structure are determined.

1:51PM B23.00014 Magnesium phase diagrams: Have you seen us? . GUS HART, Brigham Young University. STEFANO CURTAROLO, Duke University — Because of it’s high strength-to-weight ratio, magnesium is seen as promising material for automotive applications. But magnesium alloys are far less understood that more common alloys such as steel or newer alloys such as aluminum. Even among simple binary magnesium systems, there is a great deal of missing information. There are binary magnesium systems for which no phase diagrams appear in the latest databases (the Pauling File, for example). Using a high-throughput approach, we have undertaken a broad search for ground states in 40 magnesium binary systems using more than 8000 fully-relaxed first-principles calculations. We find new, non-obvious ordering systems and many systems where there are unsought ground states. We discuss the results and their potential impact on magnesium alloys.

2:03PM B23.00015 First-principles thermodynamics of point defects and off-stoichiometry in $\beta$-Mg$_{17}$Al$_{12}$. DONGWON SHIN, CHRISTOPHER WOLVERTON, Northwestern University — The mechanical strength of Mg-Al alloys may be enhanced by a finite spatial dispersion of $\beta$-Mg$_{17}$Al$_{12}$ precipitates. Native point defects, i.e. vacancies and anti-sites, in Mg$_{17}$Al$_{12}$ are important for understanding the phase stability and unusually asymmetric observed off-stoichiometry in this precipitate phase. In an effort to provide a quantitative picture of the phase stability of this system, we have performed a series of first-principles density functional theory calculations of bulk and defect properties of Mg$_{17}$Al$_{12}$. We consider not only the T=0K static energetics, but also key entropic terms such as the configurational and vibrational entropies. The vibrational entropies are calculated from DFT via the direct force-constant approach using the quasiharmonic approximation. We investigate the effect of atomic vibrations on native point defect free energies of Mg$_{17}$Al$_{12}$ and combine the entropic contributions with the point defect formation energies to evaluate the thermodynamics of off-stoichiometry in this phase. We find there is a large vibrational entropy difference between Mg-rich and Mg-deficient defects in Mg$_{17}$Al$_{12}$, consistent with the strong asymmetry in the observed Mg-Al phase diagram.

Monday, March 16, 2009 11:15AM - 2:15PM –
Session B24 DMP: Focus Session: Nanotube Characterization 326

11:15AM B24.00001 Raman spectroscopy of individual freestanding single-walled carbon nanotubes of defined chiral structure. JEAN-LOUIS SAUVAJOL, University of Montpellier — We review the main information that we have obtained from Raman spectroscopy experiments combined with electron diffraction experiments on individual freestanding single-walled carbon nanotubes. This information concerns: the radial breathing mode vs diameter relationship; the dependence of the frequency and lineshape of the G-modes in semiconducting and metallic tubes; the evaluation of the optical transition energies for individual freestanding SWNTs. These experimental Raman results obtained on well-identified individual SWNTs are compared with other experimental data and theoretical predictions. From these data, we can define Raman criteria that allow identifying carbon nanotubes from their Raman features only. We show the efficiency of this approach: (i) to assign the (n,m) indices of individual freestanding single-walled carbon nanotubes, and (ii) to identify the (n,m) tubes organized in a small bundle.

11:51AM B24.00002 Raman Studies of Exciton and Exciton-Phonon Coupling Behavior in Metallic Single-Walled Carbon Nanotubes. STEPHEN DOORN, Los Alamos National Laboratory — A scaling law analysis of carbon nanotube transition energies has been found to be valuable in revealing new electronic behaviors for the third and fourth transitions in semiconducting nanotubes. In the work presented here, we discuss resonance Raman data obtained for the $E_{22}^{11}$ and $E_{22}^{12}$ transitions of a broad diameter range (0.7 - 4 nm) of metallic carbon nanotubes. We show that application of the scaling law analysis to transition energies for metallic nanotubes suggests that the transitions are excitonic in nature and that relative scaling of electron self-energies and exciton binding energies in metallic nanotubes closely matches that found in semiconductors. This similarity in behavior can be understood in terms of similar regions of the Brillouin zone being sampled by $E_{22}^{11}$ and $E_{22}^{12}$ and by $E_{22}^{44}$ and $E_{22}^{45}$. Additionally, for large diameter nanotubes (> 1.3 nm) we now observe the previously elusive upper branch signatures for several chiralities for both $E_{22}^{12}$ and $E_{22}^{11}$ excitation. These results are discussed as a consequence of the nodal behavior of exciton-phonon coupling. Also, while theoretical calculations for the (n,m)-dependent matrix elements predict the RBM intensity should decrease with increasing diameter; the opposite behavior is observed experimentally. We show this to be a consequence of an increase in the resonance Raman broadening factor $\Gamma$ as diameter decreases. Finally, we present Raman excitation data from surfactant suspensions highly enriched in metallic nanotubes via density gradient ultracentrifugation. Specifically, we will focus on the evolution of G-band behavior over a wide range of chiralities enabled by these new sample types. The variable behavior of the Breit-Wigner-Fano line in these enriched ensemble samples will be discussed.
ERIK HAROZ, WILLIAM RICE, BENJAMIN LU, Department of Electrical and Computer Engineering, Rice University, ROBERT HAUGE, Department of Chemistry, Rice University, DONNY MAGANA, STEPHEN DOORN, Chemistry Division, Los Alamos National Laboratory, PASHA NIKOLAEV, SIVARAM AREPALLI, Johnson Space Center, National Aeronautics and Space Administration, JUNICHIRO KONO, Department of Electrical and Computer Engineering, Rice University — We performed resonance Raman spectroscopy studies of metallic single-walled carbon nanotubes (SWNTs), including armchair SWNTs from (6,6) through (10,10). The measurements were carried out with excitation of 440-850 nm on aqueous ensemble samples of SWNTs enriched in metallic species. From this, we generated Raman excitation profiles (REFs) of the radial breathing mode and compare the REFs of armchairs and other metallic species. Additionally, we measured REFs of the G-band mode and observed how the Breit-Wigner-Fano line shape of the G- peak evolves in peak position, width and intensity relative to the G+ peak as different metallic nanotubes are excited. By combining these studies with absorption and photoluminescence excitation spectroscopy studies, we present a comprehensive examination of the optical signatures of metallic SWNTs.

HUGEN YAN, DAOHUA SONG, TONY HEINZ, Columbia University — Time-resolved Raman spectroscopy has been applied to determine the population lifetime of both zone-center and zone-edge optical phonons. Non-equilibrium populations of these phonons were produced by the rapid release of charge carriers following photooxidation of the nanotube sample with a femtosecond laser pulse. The temporal evolution of these phonon populations was recorded using the strength of anti-Stokes Raman scattering in G-mode (for the zone-center phonons) and D-mode (for the zone-edge phonons) as a function of the time delay of the fs probe pulse. A longer lifetime was found for the D-mode than for the G-mode phonons, a result consistent with recent ab-initio calculations of the anharmonic decay of these phonons [1]. We also report on the transient mode populations for the zone-center and zone-edge phonons that result from carrier cooling. [1] N. Bonini, M. Lazzeri, N. Marzari, and F. Mauri, Phys. Rev. Lett. 99, 176802 (2007).

12:51PM B24.00005 Investigation of Nanotube Growth Mechanisms via In-Situ Spectroscopy  
HAUL RAO, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFFL/RX, WPAFB, OH 45433, UTC Inc., Dayton, OH 45432, DAVID LIPTAK, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFFL/RX, WPAFB, OH 45433, UES Inc., Dayton, OH 45432, ROBERTO ACOSTA, BENJI MARUYAMA, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFFL/RX, WPAFB, OH 45433, AFFL TEAM — Analysis of single-walled carbon nanotubes (SWNTs) during growth via Raman spectroscopy offers a unique approach to understand their growth mechanism, which remains unclear due to large variations of parameters in synthesis methods. In our technique the SWNTs are synthesized via chemical vapor deposition inside an environmental cell coupled to an automated stage. Growth occurs from catalyst nanoparticles on thermally isolated islands within substrates. In-situ micro-Raman spectroscopy performed on zone-center (G band) and zone-edge (D band) of low-pressure CNTs where the excitation laser also serves as a localized heat source for CNT growth. Control over substrate temperature and position, feed gas composition, and chamber pressure enable rapid real-time exploration of SWNT growth parameter space. Comparison of nanotube nucleation and growth kinetics from various metallic catalytic particles will be presented and implications for nanotube catalyst design will be discussed.

1:03PM B24.00006 Characterisation of Carbon Nano-Materials with the Confocal Raman AFM  
KLAS WEISHAUP, THOMAS DIEING, MATTHIAS KRESS, UTE SCHMIDT, WITec GmbH, Ulm, Germany — Graphene and carbon nanotubes represent perfect model systems for fundamental research. Carbon nanotubes have proven to be unique systems for the study of Raman spectra in one-dimensional systems. Raman spectroscopy has proved to be one of the most powerful techniques for characterizing single walled carbon nanotubes in terms of chirality, diameter, and electronic states. The 2D peak evolves in peak position, peak intensity and width in a characteristic matter of the electronic states. Proximity of the electronic states to the Fermi level changes the 2D peak position and width. We present results on the chirality dependent material evolution for both graphene and carbon nanotubes. The influence of the different synthesis methods is discussed. The strong phonon coupling of graphene is discussed and compared to the electronic excitations. The detected peaks are explained using a joint photoemission and Raman spectroscopy analysis.

1:15PM B24.00007 Resonance Raman Scattering for Quantification of the Bundling of SWNTs  
TAO LIU, ZHIWEI XIAO, High Performance Materials Institute, Florida State University — The strong attractive van der Waals interaction induces individual SWNTs to form bundles or ropes. It has been demonstrated both experimentally and theoretically that, the various physical properties of SWNTs, e.g., photoluminescence, and electronic, and mechanical, strongly depends upon their bundling states. Upon comparative studies of SWNT dispersions with the preparative ultracentrifuge method, which is a newly developed characterization technique by us for quantifying the structures of SWNTs in a dispersion, and resonance Raman scattering, we demonstrate that the bundling states for a given SWNT dispersion can be quantified with the latter technique. In this presentation, the preparative ultracentrifuge method for studying the processing-structure-property relationships of SWNT dispersion will be introduced. The mechanisms of using resonance Raman scattering to quantify the bundling states of SWNTs will be discussed.

1:27PM B24.00008 ABSTRACT WITHDRAWN —

1:39PM B24.00009 Electrical Characterization of Carbon Nanotube Bundles Synthesized from Chemical Vapor Deposition of Ferrocene  
C. WOLFE, R. SHAH, Z. ZHANG, Department of Physics, Southern Illinois University Carbondale, Illinois, 62901, X. AN, S. KAR, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, S. TALAPATRA, Department of Physics, Southern Illinois University Carbondale, Illinois, 62901 — We employed a chemical vapor deposition technique, which used ferrocene both as the catalyst as well as the carbon source, to grow films of carbon nanotubes (CNT). The CNT films obtained using this procedure were characterized using Raman Spectroscopy and Transmission Electron Microscopy which indicated the presence of thin diameter carbon nanotubes as well as single walled CNT ropes. Electrical transport measurements performed on long ropes of CNTs extracted from these bulk films will be presented and will be discussed in the framework of transport theories of quasi-one dimensional systems.

1:51PM B24.00010 Coherent Phonon Dynamics in Single-Walled Carbon Nanotubes  
L.G. BOOSHEHRI, E.H. HAROZ, J. KONO, Rice University, Y.S. LIM, Konkuk University, J.H. KIM, K.J. YEE, Chungnam National University, G.D. SANDERS, C.J. STANTON, University of Florida — Understanding how electrons and phonons relax in energy and momentum is one of the current goals in carbon nanotube spectroscopy as well as an important step towards developing novel electronic and optoelectronic devices based on carbon nanotubes. Recent ultrafast pump-probe spectroscopy studies of single-walled carbon nanotubes (SWNTs) have successfully detected coherent phonon dynamics, but the dominant dephasing mechanism that occurs with decoherence of phonon mode oscillation has yet to be understood. Our present work demonstrating ultrafast coherent phonon spectroscopy of the radial breathing mode (RBM) of semiconducting SWNTs provided a powerful method for determining phonon energies in an ensemble of SWNTs. We now extend our previous studies to provide new insight into the dephasing mechanisms of coherent phonons in SWNTs. Here, we systematically investigated the temperature, polarization, and wavelength dependence of coherent phonon dephasing times, amplitude, and frequency for various types of nanotube film and solution samples.
The work was supported by NSF, DOE, the Welch Foundation, and NSFC.
Excitonic supersolid in quantum Hall graphene bilayers, YOGESH JOGLEKAR, Indiana University-Purdue University Indianapolis (IUPUI), CHANG-HUA ZHANG, Kansas State University — We study the ground state of two graphene sheets separated by a distance $d$ in the quantum Hall regime where the top layer has electrons and the bottom layer has holes as carriers. We obtain a rich mean-field phase diagram as a function of distance $d$ and the filling factor $\nu = \nu_h = \nu$ for different Landau levels. We find that the ground state in high Landau levels at large $d$ is a generalized Wigner crystal that includes anisotropic stripe and bubble states, and at small $d$ the ground state is an uniform excitonic condensate. We show that for a wide range of partial filling factors $0 \leq \nu \leq 1/2$, at intermediate values of $d$, the ground state has interlayer phase coherence as well as a lattice structure, i.e. it is an excitonic supersolid. We discuss the predictions for signatures of such a state in transport and optical experiments.

This work was supported by IUPUI Research Support Fund Grant

Transport on quantum antidot made of 4-terminal graphene ribbons, ANDREA LATGE, CARLOS RITTER, UFF-Instituto de Física, PEDRO ORELLANA, UCN-Departamento de Física, MONICA PACHECO, UTSM-Departamento de Física — Electronic and transport properties of four-terminal graphene ribbons are discussed taking into account different configurations of quantum antidot potentials, designed at a central conductor. In general, the formation of these antidot potentials promotes a reorganization of the carriers, leading to an electronic localization at the neighboring vacancy sites. Depending upon the position, extension, and symmetries of such antidots, one may find delocalization along the structure due to the formation of new allowed paths. Here we discuss the origin of conductance dips, maximum and complete transport suppressions, within the microscopic scenario of the electronic localization, and using real-space Green function formalism. For such analysis we construct local electronic density of states mapping for different antidot configurations. The results are discussed in comparison with equivalent two-lead devices and perfect structures.

Gate-field effect in multilayer graphenes, MIKITO KOSHINO, Tokyo Institute of Technology — We study the electronic properties of the multilayer graphenes in presence of the external electric field perpendicular to the layers. We calculate the electronic potential of each layer taking account of the screening effect, to obtain the self-consistent band structure within the effective mass approximation. We calculate the conductivity using the self-consistent Born approximation and analyze its external-field dependence for every layer number. We also compute the optical absorption spectra, which is found to be strongly modified by the electric field.

Chemical Doping and Electron-Hole Conduction Asymmetry in Graphene Devices, ROKSANA GOLIZADEH MOJARAD, Purdue University, DAMON FARMER, VASILI PEREBEINOS, YU-MING LIN, GEORGE S. TULEVSKI, JAMES C. TSANG, ALI AZALI, PHAEDON AVOURIS, IBM T.J. Watson Research Center — We investigate polyethylene imine and diazonium salts as stable, complementary dopants on graphene. Transport in graphene devices doped with these molecules exhibits asymmetry in electron and hole conductance. The conductance of one carrier is preserved, while the conductance of the other carrier decreases. Simulations based on nonequilibrium Green’s function formalism suggest that the origin of this asymmetry is imbalanced carrier injection from the graphene electrodes caused by misalignment of the electrode and channel neutrality points.

Sub-lithographic Patterning of Extended Arrays of Graphene Nanostructures, KE LI, 1, WEI HAN, 2, SARAH C. PARKS, 1, WENZHONG BAO, JOHN CIRALDO, CHUN NING LAU, ROLAND KAWAKAMI, 2, EZEKIEL JOHNSTON-HALPERIN, 1 (1 Department of Physics, The Ohio State University; 2 Department of Physics and Astronomy, University of California, Riverside) — Quasi-one-dimensional graphene nanoribbons (GNRs) with narrow width ($w \leq 10$ nm) and smooth edges have been shown to exhibit bandgaps due to quantum confinement and edge effects. Current fabrication methods of GNRs include electron beam lithography and chemical synthesis. However, the lithographic approach has difficulties in reaching true nanometer-scale widths while the chemical approach lacks fidelity in GNR length and width control. The recent development of sub-lithographic patterning using the superlattice nanowire pattern transfer (SNAP) technique provides a novel approach to fabricating ultra-long graphene arrays with N

Gate-field effect in multilayer graphenes, MIKITO KOSHINO, Tokyo Institute of Technology — We study the electronic properties of the multilayer graphenes in presence of the external electric field perpendicular to the layers. We calculate the electronic potential of each layer taking account of the screening effect, to obtain the self-consistent band structure within the effective mass approximation. We calculate the conductivity using the self-consistent Born approximation and analyze its external-field dependence for every layer number. We also compute the optical absorption spectra, which is found to be strongly modified by the electric field.

Quantum Hall edge transport across graphene monolayer-bilayer junctions, YUE ZHAO, Graduate Student, Physics Department Columbia University, MIKITO KOSHINO, Research Associate, Tokyo Institute of Technology, PHILIP KIM, Associate Professor, Physics Department, Columbia University — We experimentally studied the transport property of a graphene monolayer-bilayer junction in the Quantum Hall (QH) regime. Both the monolayer graphene (MG) and the bilayer graphene (BG) develop their own landau levels under high magnetic field. While the transport measurement shows their distinct QH effect in bulk part of the MG and BG respectively, the transport measurement across the interface exhibits unusual transverse transport behaviors. The transverse resistance across the MG BG interface is asymmetric for opposite sides of the hall bar, and its polarity can be changed by reversing the magnetic field direction. When the QH plateaus of MG and BG overlap, quantized resistance will appear only on one side of the hall bar electrode pairs across the junction. These experimental observations can be ascribed to the QH edge state transport across the MG/BG interface.

Dissipation and Criticality in the Lowest Landau Level of Graphene, PALLAB GOSWAMI, Rice University, XUN JIA, SUDIP CHAKRAVARTY, UCLA — The lowest Landau level of graphene is studied numerically by considering a tight-binding Hamiltonian with disorder. The Hall conductance $\sigma_{xy}$ and the longitudinal conductance $\sigma_{xx}$ are computed. We demonstrate that bond disorder can produce a plateaulike feature centered at $\nu = 0$, while the longitudinal conductance is nonzero in the same region, reflecting a band of extended states between $\pm E_c$, whose magnitude depends on the disorder strength. The critical exponent corresponding to the localization length at the edges of this band is found to be $2.47 \pm 0.04$. When both bond disorder and a finite mass term exist the localization length exponent varies continuously between $\sim 1.0$ and $\sim 7/3$.

Session B26 DMP DCOMP: Focus Session: Computational Nanoscience II: Mechanics, Dynamics, and Assembly
11:15AM B26.00001 An atomistic approach to viral mechanical oscillations, OTTO F. SANKEY, Arizona State University — Viruses are the simplest “life” form. These parasites reproduce by borrowing the machinery of their host cell. Many are pathogenic to plants, animals, and humans. Viruses possess an outer protein coat (capsid) that protects its genomic material that resides inside. We have developed a theoretical technique to model the very low frequency mechanical modes of the viral capsid with atomic resolution. The method uses empirical force fields and a mathematical framework borrowed from electronic structure theory for finding low energy states. The low frequency modes can be “pinged” with an ultra-short laser pulse and the aim of the light/vibrational coupling is to interfere with the viral life cycle. The theoretical work here is motivated by the recent work of Tsen et al. [2] who have used ultra-short pulsed laser scattering to inactivate viruses. The methodology can be applied to many systems, and the coupled mechanical oscillations of other floppy biomolecules such as a complete ATP binding cassette (ABC transporter) will also be discussed. Co-authors of this work are Dr. Eric Dykeman, Prof. K.-T. Tsen and Daryn Benson.


11:51AM B26.00002 A new paradigm for self-assembly: The role of reversibility in viral capsid growth, DENNIS RAPAPORT, Bar-Ilan University — The phenomenon of supramolecular self-assembly, despite its importance, remains an enigma. The formation of virus capsids — the exquisitely designed protein shells of spherical viruses — is a well-known example, and there are numerous potential applications for nanotechnology. The capsid assembly process can be modeled using molecular dynamics simulation of simplified particles that are designed to form polyhedral shells. New insights into the mechanism of self-assembly have emerged from simulations carried out using particles immersed in an explicit solvent. Contrary to expectation, self-assembly is found to proceed via a cascade of strongly reversible steps, a feature that helps avoid growth-impeding kinetic traps because partial shells generally tend to lose rather than gain members. This ensures a robust process leading, under suitable conditions, to a high yield of complete shells. Furthermore, despite the large variety of possible intermediate structures, the assembly pathways are found to involve only a small fraction of highly bonded (low energy) forms.

12:03PM B26.00003 Calculation of the free energy of binding of DNA bases on a single-wall carbon nanotube, ROBERT JOHNSON, A.T. CHARLIE JOHNSON, MICHAEL KLEIN, University of Pennsylvania — Molecular bases can be combined with inorganic nanostructures to form multifunctional hybrid materials with unique properties that will drives advances in nanoelectronics, environmental safety, medicine and homeland security. One such material of contemporary interest is the DNA-carbon nanotube hybrid (DNA-CN), which consists of a single-wall carbon nanotube (SWCN) coated with a self-assembled monolayer of single-stranded DNA (ssDNA). Computation and experiment indicate that DNA-CN self-assembles with DNA bases using an energy minimization technique, “binary hierarchical assembly.” To address these issues and expand our understanding of DNA-CN, we have computed the binding free energy of individual DNA bases with SWCN using alchemical free energy methods. Such calculations provide detailed information about the importance of electrostatic, van der Waals and hydrophobic interactions in base-SWCN binding.

1This work was supported by JSTO, DTRA and the Army Research Office Grant # W911NF-06-1-0462.

12:15PM B26.00004 Simulations of the self-assembly of CdTe nanoparticles into large pitch helices, AARON SANTOS, SUDHANSHU SRIVASTAVA, SHARON GLOTZER, NICHOLAS KOTOV, University of Michigan — Recent experiments have shown that CdTe nanoparticles can self-assemble into wires, sheets, or helical nanoribbons with a large pitch length (300-400 nm) depending on the amount and type of capping group used. While conventional Monte Carlo simulations of electronically charged truncated tetrahedrons successfully predict the formation of wires and sheets, they are inadequate to describe the formation of helical nanoribbons, which require a large number of particles and a long run time to observe their characteristic features. We use a newly developed energy minimization technique, “binary hierarchical assembly,” to predict the packing structure of tetrahedral CdTe nanoparticles within the helix. From this packing structure, we construct nanoribbons of various widths and minimize the energy to determine the width of the stable structure. We find the stable width of the ribbon is charge dependent with values that correspond to ribbons observed in experiments.

12:27PM B26.00005 Sensitivity Limits of Nanomechanical Resonance Spectroscopy, P. ALEX GREANEY, U.C. Berkeley — The sensitivity limit of the recently proposed chemical sensing method, nanomechanical resonance spectroscopy (NRS) [2] is investigated using classical molecular dynamics simulations. The NRS method exploits the preferential transfer of energy between resonant modes, using an array of nanomechanical resonators to interrogate the vibrational spectrum of an analyte directly. We report on the effects of solvent and complex analytes.


12:39PM B26.00006 Enhancing Molecular Dynamics to Capture Electronic Effects, N.A. MODINE, R.E. JONES, D.L. OLMSTED, J.A. TEMPLETON, Č.J. WAGNER, Sandia National Laboratories, R.M. HATCHER, Lockheed Martin Advanced Technology Laboratories, M.J. BECK, Vanderbilt University — In modeling non-equilibrium thermal transport in nanoscale systems, classical molecular dynamics (MD) has the primary strength of explicitly representing phonon modes and scattering mechanisms. On the other hand, electrons and their role in energy transport are missing. Our goal is to couple a MD treatment of the ionic subsystem with a partial differential equation based model of the electronic subsystem in order to accurately capture aggregate behavior at the nanoscale. Along these lines, we have enhanced the LAMMPS MD package by coupling the ionic motions to a finite element based representation of electronic heat transport. The coupling between the subsystems occurs via a local version of the two-temperature model. Key parameters describing the coupling are calculated using Time Dependent Density Functional Theory (TDDFT) calculations with either explicit or implicit energy flow. We will discuss initial demonstrations of our approach focusing on nanowires and carbon nanotubes.


12:51PM B26.00007 Rotary molecular motion at the nanoscale: motors, propellers, wheels, LELA VUKOVIC, BOYANG WANG, PETR KRAL, University of Illinois at Chicago — We describe by molecular dynamics simulations nanoscale systems that could realize rotary motion. First, we study molecular propellers formed by carbon nanotube rotors with attached aromatic blades [1]. We show that these propellers could pump different types of liquids, and their pumping efficiency strongly depends on the chemistry of the (hydrophobic or hydrophilic) liquid-blade interactions in base-SWCN binding.

rate Interfaces

Several rounds of pumping were simulated to achieve more continuous flow of fluid through the nanotube. Pressure difference in different regions was analyzed.

We present molecular dynamics simulations of carbon nanotubes that were embedded in liquid argon. The fluid was pushed through the nanotubes to study the phenomena of nanofluidics. The previous modeling and simulation efforts were based on diffusion of atoms or molecules that were thrown to the nanotubes with initial velocities. However, we find that these functionalized coatings affect the interactions between nanoparticles and with the surrounding solvent. Thus, we present results from a series of molecular dynamics simulations of polyethylene oxide (PEO) coated silica nanoparticles of varying size (5 to 20 nm diameter) in water. For a single nanoparticle, we determined the Stokes drag on the nanoparticle as it moves through the solvent and as it approaches a wall. Due to hydrodynamic interactions, there are large finite size effects which we estimate by varying the size of the simulation cell. We also determined both solvent-mediated (velocity-independent) and lubrication (velocity-dependent) forces between two nanoparticles as a function of the coverage and chain length of the PEO chains.

Flow can be accurately described in terms of continuum mechanics and the enhancement agrees with predictions from the slip-modified Hagen-Poiseuille flow. The observed flow rate to that predicted from the no-slip Hagen-Poiseuille relation, is calculated for each CNT. In CNTs with diameters greater than 1.39 nm, the flow rate is predicted to be directly proportional to the inverse of the particle radius due to the Gibbs-Thomson effect. However, the depression of the nucleation temperature during heating was investigated using a molecular dynamics simulation. A nucleus was generated near one side of the particle and solidification spread toward the other side during nucleation process. On the other hand, the surface melting and subsequent inward melting of the solid core of the nanoparticles were observed during heating. The depression of the melting point was proportional to the inverse of the particle radius due to the Gibbs-Thomson effect. However, the depression of the nucleation temperature during cooling was not monotonic with respect to the particle radius since the nucleation from an undercooled liquid droplet was observed during cooling in all nanoparticles considered. A nucleus was generated near one side of the particle and solidification spread toward the other side during nucleation process. On the other hand, the surface melting and subsequent inward melting of the solid core of the nanoparticles were observed during heating.

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This work was supported by the NSF under Grant No. 0510163

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1:03PM B26.00008 Long-Range Hydrodynamic Interactions Implemented into LAMMPS (Parallel MD), FRANCES MACKAY, COLIN DENNISTON, University of Western Ontario — We use an explicit solvent method to study the interaction between particles and a fluid. Similar to the Particle-Mesh-Ewald schemes for electrodynamics, the long range hydrodynamic interactions are treated by interpolating the particle density onto a mesh. This is then coupled to the fluid, which we model using a thermal lattice Boltzmann scheme. Mass and momentum conserving noise in the lattice Boltzmann fluid scheme provides a thermostat for both the fluid and the particles. This work has been fully parallelized and implemented into LAMMPS, an open-source molecular dynamics code. We demonstrate the scheme with some examples from colloidal physics and flow over rough surfaces.

1:15PM B26.00009 Atomic Simulations of Hydrodynamic and Interaction Forces on Functionalized Silica Nanoparticles, J. MATTHEW D. LANE, AHMED E. ISMAIL, MICHAEL CHANDROSS, Sandia National Labs, CHRISTIAN D. LORENZ, King’s College London, GARY S. GREST, Sandia National Labs — It is often desired to prevent the flocculation and phase separation of nanoparticles in solution. This can be accomplished either by manipulating the solvent or by tailoring the surface chemistry of the nanoparticles. We have carried out functionalization with a monolayer of oligomer chains. Since it is not known how these functionalized coatings affect the interactions between nanoparticles, we present results from a series of molecular dynamics simulations of polyethylene oxide (PEO) coated silica nanoparticles of varying size (5 to 20 nm diameter) in water. For a single nanoparticle, we determined the Stokes drag on the nanoparticle as it moves through the solvent and as it approaches a wall. Due to hydrodynamic interactions, there are large finite size effects which we estimate by varying the size of the simulation cell. We also determined both solvent-mediated (velocity-independent) and lubrication (velocity-dependent) forces between two nanoparticles as a function of the coverage and chain length of the PEO chains.

1:27PM B26.00010 Water Flow in Carbon Nanotubes: Transition from Continuum to Sub-continuum Transport, JOHN THOMAS, ALAN MCGAUGHEY, Carnegie Mellon University — Water flow through carbon nanotubes (CNTs) with diameters ranging from 0.83 nm to 4.98 nm is examined using molecular dynamics simulation. A reflecting particle membrane is used to drive the flow and the relationship between the axial pressure gradient, CNT diameter, and volumetric flow rate is examined. The flow enhancement, defined as the ratio of the observed flow rate to that predicted from the no-slip Hagen-Poiseuille relation, is calculated for each CNT. In CNTs with diameters greater than 1.39 nm, flow can be accurately described in terms of continuum mechanics and the enhancement agrees with predictions from the slip-modified Hagen-Poiseuille flow relation. In CNTs with diameters smaller than 1.39 nm, we find that the liquid structure varies with CNT diameter and a continuum-based description of the fluid flow is inappropriate. The flow enhancement for these CNTs do not agree with predictions from the slip-modified Hagen-Poiseuille flow relation. They can, however, be correlated to the diameter-specific liquid structure.

1:39PM B26.00011 Fluid flow through carbon nanotubes: a new modeling and simulation approach, MICHAEL A. AVON, Department of Mechanical Engineering, The University of Akron, ALPER BULDUM, Department of Physics, The University of Akron — The flow of fluids through carbon nanotubes was investigated in order to get a better understanding of the unique properties and phenomena of nanofluidics. The previous modeling and simulation efforts were based on diffusion of atoms or molecules that were thrown to the nanotubes with initial velocities. Here, we present molecular dynamics simulations of carbon nanotubes that were embedded in liquid argon. The fluid was pushed through the nanotubes using a moving wall piston of graphene. Single-walled, double-walled, rigid and relaxed nanotubes in different diameters were considered. In order to achieve more continuous flow of fluid through the nanotubes, several pumping rounds were simulated. Pressure difference in different regions was analyzed.

1 Supported by ODOD, Third frontier RCP

1:51PM B26.00012 Accelerated Molecular Dynamics Simulation on Friction of Incommensurate Interfaces, WOO KYUN KIM, The University of Michigan, MICHAEL FALK, The Johns Hopkins University — We apply a molecular dynamics (MD) methodology to study the friction of incommensurate interfaces. While the traditional Tomlinson model assumes a single, repeatable transition, the sliding at the real incommensurate interface is comprised of a multitude of transition modes. This may account for recent Atomic Force Microscope (AFM) experimental results that indicate more complex temperature and velocity dependence of friction that deviate from the Tomlinson predictions. Conventional MD simulations are unable to simulate a wide range of sliding rates due to time scale limitations. In this study, we achieve decreases in the simulated sliding velocity by several orders of magnitude compared with conventional MD simulations using Voter’s hyperdynamics scheme. This method uses a biased potential to reduce the barrier heights of the original potential to decrease the simulated time between slip events. The decrease in the sliding velocity makes it possible to see the atomic level processes during sliding speeds much closer to the experimental time scale. We carefully analyze the simulation results to elucidate the transition mechanisms.

This work was supported by the NSF under Grant No. 0510163

2:03PM B26.00013 Molecular dynamics study of the phase transition in the bcc metal nanocrystals, YASUSHI SHIBUTA, TOSHIO SUZUKI, The University of Tokyo — The phase transition between liquid and solid phases in bcc metal nanoparticles was investigated using a molecular dynamics simulation. The nucleation from an undercooled liquid droplet was observed during cooling in all nanoparticles considered. A nucleus was generated near one side of the particle and solidification spread toward the other side during nucleation process. On the other hand, the surface melting and subsequent inward melting of the solid core of the nanoparticles were observed during heating. The depression of the melting point was proportional to the inverse of the particle radius due to the Gibbs-Thomson effect. However, the depression of the nucleation temperature during cooling was not monotonic with respect to the particle radius since the nucleation from an undercooled liquid droplet depends on the event probability of an embryo or a nucleus.

11:15 AM B27.00001 Controlling electric fields spatially by graded metamaterials\(^1\), KIN-WAH YU, Chinese University of Hong Kong. — The local electric field of a metal-dielectric composite cylinder, whose complex permittivity is given by a spatially dependent Drude model, has been derived analytically in terms of hypergeometric functions. Our results show that the electric field inside the cylinder can be confined to any desired position. Thus one can achieve the control of electric fields by fabricating graded metamaterials with specific material parameters. The enhanced nonlinear optical response of the composite cylinder has also been calculated [1]. The results suggest that the gradation-controlled electric field distribution may be a consequence of a combination of surface plasmon resonance and the microgeometry in graded metamaterials. Moreover, such a gradation-controlled field distribution serves as a physical mechanism for understanding the enhanced nonlinear optical responses with a broad surface plasmon band [2].

\(^1\)Work supported by General Research Fund of Hong Kong SAR Government.

11:27 AM B27.00002 Terahertz nanogap antenna detection of nano-bridges and nano-rods, H.R. PARK, M.A. SEO, J.S. KYOUNG, S.M. KOO, Seoul National University, O.K. SUWAL, S.S. CHOI, Sunmoon University, N.K. PARK, D.S. KIM\(^1\), Seoul National University, CENTER FOR SUBWAVELENGTH OPTICS TEAM. — We have measured transmission properties of a composite structure consisting of nano-rods on a long (\(a_0=300\) micron) nanogap (70 nm) on Au film in broad frequency range of 0.1 THz to 1.0 THz using THz time-domain spectroscopy. The normalized transmittance with no nano-bridge or nanorod structure in the middle shows a half-wavelength resonance: the resonance frequency is \(c/(2a_n)\) where \(n\) is the index of refraction of the substrate. The nano-size bridge at the center of the nano gap gives changes the resonance characteristics profoundly, because in essence, the length \(a_n\) now halves. Mostly the same resonance-changing behavior is expected with a nano rod structure fabricated by Pt-deposition method using a focused ion beam (FIB). This small rod also acts as a bridge dividing the length of the rectangle. We also positioned nano-rods to lie at one third of each nano gap, dividing the length by the ratio of 1:2. A resonance peak shift was observed. The structure dependent resonance allows to detect nano-size particles and to tailor resonance characteristics with feature sizes of \(\lambda/10\,000\).

\(^1\)corresponding author

11:39 AM B27.00003 Terahertz Nanogap Plasmonics: Giant Field Enhancement, M. A. SEO, H. R. PARK, S. M. KOO, O. K. SUWAL, S. S. CHOI, N. K. PARK, D. S. KIM, CENTER FOR SUBWAVELENGTH OPTICS TEAM. — We show that a nanogap dividing two conducting planes can efficiently transmit terahertz electromagnetic waves with wavelengths in the millimeter range. Terahertz time domain spectroscopy is performed to probe transmittance over a frequency range of 0.1 THz to 1.5 THz. It was found that the transmittance continues to increase as the frequency decreases with a dependence of 1/f. The area-normalized transmittance, which is equivalent to the level of field enhancement, reaches the value of 800 at 0.1 THz for a sample with a 70 nm gap. Combined with the 1/f dependence, this indicates that strong local resonance is not a prerequisite for a large field enhancement. It is shown that the accumulation of charges at metal edges via light-induced currents creates a large horizontal electric field, which in effect attracts the incoming light. The enhanced field in the gap fully scatters towards the far-field because there exists no cut-off. With the broad 1/f spectral response, this structure can be an excellent launching pad for inducing terahertz nonlinearity, nano-particle detection, and for surface enhanced Raman scattering.

11:51 AM B27.00004 Active Control of Propagating Surface Plasmons Excited by a Quantum Cascade Laser\(^1\), DANIEL WASSERMAN, TROY RIBAUDO, UMass Lowell, ERIC SHANER, Sandia National Labs, SCOTT HOWARD, Cornell University, FOW-SEN CHOA, University of Maryland Baltimore County, CLAIRE GMACHL, Princeton University. — There has been significant interest, of late, in the optical properties of subwavelength features in metallic films. For instance, resonant transmission through periodic arrays of subwavelength apertures in metallic films is seen at wavelengths determined by the periodicity of the metal film and the relative permittivity of the metal and the surrounding dielectric medium. This phenomenon is referred to as extraordinary optical transmission (EOT) and has been studied for potential applications in display and sensing technologies. Here we demonstrate the ability of an actively tunable EOT grating to control the coupling of incident coherent radiation from a dual wavelength QCL to propagating surface modes on the grating. We use a novel spatially and spectrally resolved Fourier transform infrared spectroscopy technique to image the propagating surface waves on our EOT grating, and are able to extract a plasmon propagation length from the data collected.

\(^1\)Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:03 PM B27.00005 Spatial and Spectral Investigation of Extraordinary Optical Transmission\(^1\), T. RIBAUDO, University of Massachusetts at Lowell, B.S. PASSMORE, E.A. SHANER, Sandia National Laboratories, D. WASSERMAN, University of Massachusetts at Lowell. — Extraordinary Optical Transmission (EOT), or the enhancement of light transmission through periodic arrays of sub-wavelength holes in metal films, has been investigated for its clear contradiction with conventional aperture theory, as well as for possible applications in chemical sensing and display technologies. In the visible and near-infrared spectral ranges, EOT is argued to be predominantly a result of the excitation of surface plasmon polaritons (SPPs) on metal/dielectric interfaces. Here, we report our investigations of the far-field transmission characteristics of EOT gratings designed for the mid-infrared frequency range. Using a tunable Quantum Cascade Laser, we explore the spatial and spectral dependence of the transmitted far field on the angle of incidence and the exciting frequency of the laser. We show that for frequencies coincident with the EOT maximum, little SPP propagation is observed, while laser frequencies on the high energy falling edge of the EOT peak couple to such propagating modes.

\(^1\)Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:15 PM B27.00006 Mid Infrared Beam Steering Using Plasmonic Structures, DAVID ADAMS, DANIEL WASSERMAN, University of Massachusetts at Lowell. — The interaction of electromagnetic radiation with periodic features on metal surfaces has received a great deal of attention in recent years. The far-field transmission properties of a sub-wavelength aperture can be controlled when periodic grooves are formed on the exit surface, allowing the shape and directionality of the transmitted beam to be altered. This phenomenon is a result of surface plasmon polaritons propagating along the metal surface and recoupling to photons which are phase mismatched with respect to the transmitted beam. The resulting interference pattern is dependent on the wavelength of the exciting beam, the geometry of the periodic surface structure, and the dielectric permittivity of the materials at the boundary. Here we present simulations using finite element analysis which demonstrate the steering of the beam transmitted through the metal slit as the permittivity of the surrounding material is modified.
Extraordinary Optical Absorption through Plasmonic Subwavelength Slits.

High speed photodetectors, optical lithography and recording, and biosensors.

Birefringence in Ring Resonator by Free Spectral Range and Wavelength measurement.

Optical Vortexed Transmission through a Nanoslit on the Pyramid.

Visible Far-Field Superlens for Two-Dimensional Imaging Below the Diffraction Limit.

Field dependent enhancement of the magneto-optical Kerr effect by surface plasmon resonance.


Symmetry and degeneracy in metamaterial trimers.
1:51PM B27.00014 Composite Metal-Semiconductor Metamaterials with Negative Permittivity and No Loss, A. M. Bratkovsky, E. V. Ponizovskaya, S.-Y. Wang, Hewlett-Packard Labs, Palo Alto, P. Holmström, KTH, Stockholm — Close to the resonance in a planar interface between a metal and dielectric, \( \varepsilon_{\text{metal}} \approx -\varepsilon_{\text{dielectric}} \), very tight electromagnetic field confinement results, but the tighter the confinement, invariably, the higher the propagation losses. For confinement significantly better than that of Si nanowires (~300 nm) propagation losses become prohibitively high for most interconnect applications. Also, the magnitude of \( \varepsilon_{\text{metal}} \) needs to be larger than e.g. 2 in order to interface to common dielectrics for close to resonance conditions. The most straightforward way to alleviate this situation is of course to use optical gain. We have analyzed theoretically a metamaterial, which is a mix of quantum dots (QDs) half of them pumped and half absorptive and showed that one could indeed compensate the loss. More efficient way of obtaining the \( \varepsilon < 0 \) is to use metals, and we show that a combination of silver rods, supplying the negative \( \varepsilon \) and pumped QDs, providing the gain necessary to compensate the loss in the silver rods [1].


11:15AM B28.00001 Optimizing Graphene Morphology on SiC(0001), JAMES HANNON, IBM Research Division — Many schemes to integrate graphene with microelectronics assume that reliable wafer-scale synthesis processes will be developed. One promising route to wafer-scale synthesis is to form graphene overlayers from the decomposition of SiC at high temperature. We have shown that, even at 1200 C, limited diffusion at the SiC surface leads to pit formation and a non-uniform graphene film thickness [1]. In this talk I will describe our efforts to improve both graphene domain size and thickness uniformity. One way we achieve this is by forming graphene in a background pressure of disilane, which hinders SiC decomposition. Even in rather low Si partial pressures (e.g. 1e-5 Torr), the SiC decomposition temperature can shifted several hundred degrees higher in temperature [2]. Using in situ low-energy electron microscopy (LEEM), we show that this effect can be exploited to form large graphene domains (larger than 10 um) with controlled layer thickness (e.g. 1 ML). Work performed in collaboration with R.M. Tromp.


11:51AM B28.00002 Atmospheric pressure growth of graphene on SiC(0001), THOMAS SEYLLER, University of Erlangen — Graphene, a single monolayer of sp2-bonded carbon, is a very unique 2-dimensional electron gas system with electronic properties fundamentally different to other 2DEG systems [1]. Several production routes exist for graphene. Among them, the solid-state decomposition of hexagonal silicon carbide (SiC) surfaces [2] is particularly attractive for the development of graphene based electronics [3,4]. The first part of the presentation gives a brief summary of recent studies on the structural and electronic properties of graphene and few-layer graphene grown on SiC(0001) under ultra-high vacuum (UHV) conditions. The second part of the talk is devoted to recent progress in the growth of large domain graphene films on SiC(0001) in Ar atmosphere. It is shown that growth in Ar ambient leads to a significant improvement of the surface morphology and domain size as well as carrier mobility.


12:27PM B28.00003 Centimeter scale pattern growth of graphene films for stretchable transparent electrodes, BYUNG HEE HONG, Sungkyunkwan University — Large scale pattern growth of graphene is one of the most awaiting problems to be solved in order to bring this material for device application. Recently, macroscopic scale graphene films have been prepared by two-dimensional assembly of graphene sheets chemically derived from graphite crystals and graphene oxides. However, the sheet resistance of these films is found to be much larger than theoretically expected values. Here, we report the direct synthesis of centimeter-scale graphene films utilizing chemical vapor deposition (CVD) on thin Ni layers, where the overall structures are connected by lateral electric connections. As a result, the transferred graphene films show very low sheet resistance with excellent optical transparency. At low temperatures, the single layers transferred on SiO2 substrates show high electron mobility with the signature of quantum Hall effect, implying that the quality of CVD-grown graphene is as high as mechanically cleaved graphenes. Employing these outstanding mechanical properties of graphenes, we also demonstrate the macroscopic usage of the highly conducting and transparent electrodes for flexible/stretchable/foldable electronics.

1:03PM B28.00004 Fabrication and measurement of epitaxial graphene nanoribbons, MIKE SPRINKLE, Georgia Institute of Technology, JEFF J. PETERSON, Intel Corporation, MING RUAN, YIKE HU, XIAOSONG WU, EDWARD H. CONRAD, Georgia Institute of Technology, CLAIRE BERGER, CNRS and Georgia Institute of Technology, WALT A. DE HEER, Georgia Institute of Technology — Multi-layer graphene grown epitaxially on the C-terminated (000T) surface of 4H-SiC in a low vacuum (~10~14 Torr), high temperature (~1420 °C) induction furnace environment has been shown to be of extremely high quality and mobility. Due to its rotational stacking, the material exhibits electronic properties similar to other 2D materials [1]. Several production routes exist for graphene. Among them, the solid-state decomposition of hexagonal silicon carbide (SiC) surfaces [2] is particularly attractive for the development of graphene based electronics [3,4]. The first part of the presentation gives a brief summary of recent studies on the structural and electronic properties of graphene and few-layer graphene grown on SiC(0001) under ultra-high vacuum (UHV) conditions. The second part of the talk is devoted to recent progress in the growth of large domain graphene films on SiC(0001) in Ar atmosphere. It is shown that growth in Ar ambient leads to a significant improvement of the surface morphology and domain size as well as carrier mobility.


1:15PM B28.00005 Self Assembly of Graphene Sheets, HAILIANG WANG, XIRAN WANG, XIAOLIN LI, HONGJIE DAI, Stanford University — Chemically derived graphene sheets (GS) were found to self-assemble onto patterned gold structures via electrostatic interactions between noncovalent functional groups on GS and gold. This afforded arrays of single graphene sheets on substrates, characterized by Auger, Raman and scanning electron microscopy (SEM) imaging. Self assembly was used for the first time to produce on-substrate and fully-suspended graphene electrical devices. Molecular coatings on the GS were removed by high current “electrical annealing,” which recovered the high electrical conductance and Dirac point of the GS.

1:27PM B28.00006 Homoepitaxial Diamond Growth on Planar and Non-planar Substrates Using Carbon-13 Precursors, GOPI SAMUDRALA, University of Alabama at Birmingham, SAMUEL WEIR, Lawrence Livermore National Laboratory, YOGESH VOHRA, University of Alabama at Birmingham — The growth of single crystal diamond by microwave plasma Chemical Vapor Deposition has been carried out on [100] oriented Type Ia natural diamond anvils as well as planar Type Ib synthetic diamond substrates. The effects of substrate geometry, concentrations of Carbon-13 gas precursors, nitrogen concentration in the plasma, and substrate temperatures on homoeptaxial diamond growth have been investigated. These results will be presented along with the observed changes in growth rate and surface morphology of the grown films with the variation of each parameter. We have also investigated nitrogen incorporation in diamond lattice by photoluminescence spectroscopy. Results obtained from the study on non-planar substrates have a direct impact on the growth chemistry used in the fabrication of designer diamond anvils for high pressure research.

[1] We acknowledge support from DOE Grant No. DE-FG52-06NA26168.
11:15AM B29.00001 Spin dependent scattering in all Heusler alloy CPP-GMR nano-structures for magnetic storage applications, OLEG MYRASOV, KONSTANTIN NIKOLAEV, THOMAS AMBROSE, Seagate Technology LLC — At the reduced sensor dimensions necessary for high density magnetic recording, the lower impedance of current-perpendicular- to the plane giant magnetoresistance (CPP-GMR) based read heads likely will take over the currently used tunneling MR based sensors. Main obstacle on the of realizing this transition is relatively low amplitude of the conventional CPP-GMR stacks. In this work, we investigate all-Heusler CPP-GMR spin-valves. The combination of alloys has been chosen in order to match spin states majority channel[1]. We focus on fundamentals of spin dependent interface and bulk scattering as it is affected by substitution disorder in these ternary alloys. Ab-initio electronic structure calculations employed to account for complex band structure of these ternary. We investigate interface scattering contribution within a simple model relying on the electronic band structure calculated for bulk of ferromagnetic and non-magnetic component of all Heusler CPP GMR tri-layer. We use model to investigate how to minimize impact of disorder induced states. Experimentally, these structures have been realized using conventional sputter deposition techniques and found to exhibit significant interface scattering contribution to MR signal. [1] T. Ambrose and O. Myrasov, United States Patent 6,876,522 (April 5, 2005); T. Ambrose, O. Myrasov, “Growth and Magnetotransport Properties of Thin Co2MnGe Layered Structures”, Springer Verlag Series. 2005.

11:27AM B29.00002 Sub-gap cotunneling current through a spinfull quantum dot with superconducting leads, JENS PAAKIE, BRIAN ANDERSEN, KARSTEN FLENSBERG, University of Copenhagen — A number of recent experiments have measured the voltage driven current through a quantum dot with superconducting leads. By changing the gate voltage of the dot, several unusual properties of the sub-gap current have been revealed. For example, when the dot is occupied by an odd number of electrons, the cotunneling conductance exhibits regions of negative differential conductance as well as significant weight redistributions among the multiple Andreev scattering resonances. We have calculated the sub-gap cotunneling current within a general Hamiltonian approach, allowing us to treat the even occupied (spinless) dot exactly, and the odd occupied (spinfull) dot perturbatively. In the latter case, we present calculations of unusual sub-gap current and relate these findings to the experiments.

11:39AM B29.00003 Orientation and temperature dependence of the anomalous Hall effect in hcp cobalt, JVO SOUZA, University of California, Berkeley, ERIC ROMAN, YURIY MOKROUSOV, University of California, Berkeley and University of Hamburg — We calculate from first-principles the evolution of the intrinsic anomalous Hall conductivity vector $\vec{a}$ of hcp Co as the spin magnetization direction $M$ is tilted away from the $c$-axis. We find that $\vec{a}$ varies smoothly with the tilt angle $\theta$, and that its magnitude is strongly reduced, by a factor of about four, between $\theta = 0$ and $\theta = \pi/2$, in good agreement with the measured anisotropy ratio of about three$\textsuperscript{[1]}$. In addition to the anisotropic linear magnetization dependence ($\sigma_{\parallel}/M_\parallel \neq \sigma_{\perp}/M_\perp$) expected for any uniaxial crystal, there is a considerable nonlinearity in the dependence of $\sigma_{\perp}$ on $M_\perp = M \sin \theta$, while the relation between $\sigma_{\parallel}$ and $M_\parallel = M \cos \theta$ is essentially linear, as in Mn$_2$Ge$\textsuperscript{[2]}$. The overall angular dependence of $\vec{a}$ is well-described by an expansion in terms of $l = 1$ and $l = 3$ spherical harmonics. From Zener’s model for the influence of thermal fluctuations of $M(r)$ on the temperature dependence of magnetic anisotropies$\textsuperscript{[3]}$, we predict that the $l = 3$ terms give rise to an appreciable increase with temperature of the anisotropy ratio.

11:51AM B29.00004 Determination of spin polarization of amorphous ferromagnet CoFeB by Point-Contact Andreev Reflection, SUNXIANG HUANG, TINGYONG CHEN, CHIA-LING CHIEN, The Johns Hopkins University — Amorphous ferromagnet CoFeB plays a key role in spintronic devices. Larger tunneling magnetoresistance (TMR) is resulted when amorphous CoFeB is incorporated into either AlO$_x$ or MgO magnetic tunnel junctions (MTJs) than those with CoFe. The critical switching current density in spin transfer torque devices with CoFeB as the free layer is significantly less than that with NiFe. The TMR of MgO-based MTJs are also noticeably different using Co$_{80}$Fe$_{20}$ and Co$_{40}$Fe$_{60}$B$_{20}$. These phenomena indicate a substantial spin polarization of CoFeB, whose value and compositional dependence should be determined. We have recently determined the spin polarization of amorphous Co$_{80-x}$Fe$_{8}$B$_{20}$($x=20, 40, 60$) using the point-contact Andreev reflection technique$\textsuperscript{[1]}$. The spin polarization of amorphous CoFeB has been found to be as high as 65%. In contrast to the large enhancement of TMR during crystallization of CoFeB or MgO-based MTJs, the spin polarization of crystallized CoFeB is in fact much reduced. Very recent theoretical studies$\textsuperscript{[2]}$ using density functional theory indicate an enhanced spin polarization in amorphous CoFeB, in good agreement with our measurements. [1] S. X. Huang et al., APL, 92, 242509 (2008). [2] P.V. Paluskar et al., PRL, 100, 057205 (2008).

12:03PM B29.00005 Structural and orientation dependence of the anomalous Hall effect in cobalt crystals, ERIC ROMAN, IVO SOUZA, University of California, Berkeley — Co undergoes a structural phase transition at 600 K from a ferromagnetic hcp phase to a ferromagnetic fcc phase. We present a first-principles study of the anomalous Hall conductivity (AHC) in hcp, fcc, and fct cobalt crystals. We find that the AHC in the fcc phase is about half that of the hcp phase, in good agreement with experiment. By expressing the AHC as the Kramer's-Kronig transform of the magnetic circular dichroism (MCD) spectrum, we relate the change in the AHC to differences between the infrared MCD spectra of the two phases. In particular, there is a large, negative spin-flip contribution to MCD, which is absent in hcp Co. These distortions alter the dependence of the AHC on the magnetization direction, an effect which is also significant for the orbital moment.

12:15PM B29.00006 Measurement of the transport spin polarization of disordered metals using point-contact Andreev reflection, M. OSOFSKY, Naval Research Laboratory, G. WOODS, J. SANDERS, H. SRIKANTH, University of South Florida, S. KOLESNIK, T. MAXWELL, B. DABROWSKI, Northern Illinois University — Point contact Andreev reflection (PCAR) studies were done on bulk, polycrystalline SrRu$_{1-x}$TM$_x$O$_3$ (TM = Cr, Mn, Ti) and SrRu$_{0.9}$Os$_{0.1}$O$_2$ with a high degree of disorder. The curves are typical of many other materials studied, except that the conductance is not constant at large voltages as is commonly observed in most metals. This result is most likely due to the effect of disorder on the density of states (DOS) that produces the well known square-root-of-V anomaly. After the problem of the $V^{1/2}$ behavior at large $V$ was eliminated by proper normalization, the CAR spectra for samples were analyzed using the modified BTK model. Pure SrRuO3 undergoes ferromagnetic ordering at a Curie temperature of $T_C \sim 160$ K and has a relatively high spin polarization ($\sim 0.6$). Our results indicate that, when the lattice is disordered from either the presence of Ru lattice site defects or the substitution of a transition metal for the Ru, the curie temperature, $T_C$, changes by a factor of two while the spin polarization is almost unchanged.

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12:27PM B29.00007 Anomalous Hall effect in Y$_2$Fe$_{17-x}$Co$_x$ single crystals, JOLANTA STANKIEWICZ, ICMIA, CSIC-Universidad de Zaragoza, KONSTANTIN SKOKOV, Tver State University — We study experimentally the Hall resistivity of Y$_2$Fe$_{17-x}$Co$_x$ single crystals ($x \leq 8$) for wide temperature and applied magnetic field ranges, and for various magnetic field orientations with respect to the easy-magnetization axis. We find a large anomalous Hall effect (AHE) anisotropy in this system for $x \leq 2$. The AHE resistivity $\rho_{xy}$, measured with an applied magnetic field $H \perp c$-axis, is nearly one order of magnitude larger than the one for $H$ along the hard magnetization direction ($H \parallel c$-axis). Furthermore, the former is very large and varies linearly with the longitudinal resistivity $\rho$, whereas the latter follows $\rho^2$ for $T < 150$ K. We tentatively interpret the behavior of $\rho_{xy}$ for $H \parallel c$-axis in terms of an intrinsic effect related to the inter-orbital hopping between degenerate $d$-orbitals. Such hopping is allowed for high symmetry points at the crystallographic dumb-bell sites in this configuration. On the other hand, there is no inter-orbital hopping for $H \perp c$-axis. However, a huge amplitude of the AHE resistivity for this configuration, which follows from skew scattering, is puzzling. Both the AHE anisotropy and the large skew scattering go away as more Fe is substituted by Co. We attribute this to variations in the electronic structure of the Y$_2$Fe$_{17-x}$Co$_x$ system when Co atoms start to occupy the dumb-bell crystallographic sites.

12:39PM B29.00008 Signal propagation in time-dependent spin transport$^1$, YAO-HUI ZHU, HANS CHRISTIAN SCHNEIDER, University of Kaiserslautern — Signal propagation in magnetic multilayers is studied using a macroscopic theory of time-dependent spin transport. Our analysis shows that time-dependent spin transport possesses a wave-diffusion, i.e., it is wave-like for fast signal modulation and reduces to the diffusion equation for slow modulation$^1$. The wave-like characteristics allow us to extract a finite spin signal-propagation velocity, which cannot be done using the spin diffusion equation. Applications to different switching scenarios for collinear and non-collinear spin transport through magnetic multilayers will be discussed.

$^1$Supported by the MATCOR/MAINZ programs of the state of Rheinland-Pfalz

12:51PM B29.00009 The Anomalous Hall Effect in Ultra-Thin Amorphous CNi$_3$ Films$^1$, YIMIN XIONG, PHILIP ADAMS, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001 — We present anomalous Hall (AHE) measurements in ultra-thin CNi$_3$ films. Films with sheet resistances in the range $R \ll R_Q$ to $R \sim R_Q$ were studied in fields up to 9 T and temperatures down to 2 K. We find that in addition to scattering processes, the AHE in high resistance films is strongly influenced by disorder-enhanced electron-electron interaction effects.

$^1$This work is supported by the DOE under Grant DE-FG02-07ER46420.

1:03PM B29.00010 Electronic structure and spin-filter effect of γ-Fe$_2$O$_3$ (maghemite), HIROYOSHI ITOH, Department of Pure and Applied Physics, Kansai University, Japan, SYUTA HONDA, JUN-ICHIRO INOUE, Department of Applied Physics, Nagoya University, Japan, HIDETO YANAGIHARA, EIJI KITA, Institute of Applied Physics, University of Tsukuba, Japan — We theoretically study the electronic structure and spin-dependent transport of spinel-like γ-Fe$_2$O$_3$ (maghemite) which is one of candidates for spin-filter devices. By performing first principles calculations (GGA+U) for iron vacancy ordered Fe$_{54}$O$_{96}$, the spin-dependent band-gap of the maghemite in the ferrimagnetic insulating ground state is determined. It is also shown that excess of Fe and O atoms significantly affects on the band gap of the minority spin state. In the light of obtained electronic structure, the spin-filter effect and variable range hopping of the maghemite are discussed.

1:15PM B29.00011 Scanning Probe Microscopy of Quantum Chains, ISRAEL MANDEL, GABRIEL CWILICH, FREDY ZYMPAN, Department of Physics - Yeshiva University — Quantum strongly correlated spin systems exhibit energy spectra related to their underlying classical dynamics. For integrable systems, the level-spacing is Poissonian, while for chaotic dynamics, it follows a Wigner-Dyson distribution, corresponding to localized and metallic phases$^{[1,2]}$. Linear spin chains and braids have been considered recently$^{[3]}$ showing that a certain degree of disorder or the presence of impurities along the chain induces a transition from one statistic to the other. We consider a quantum Heisenberg system of two perpendicular linear chains (T-shaped) interacting through the points of closest approach between them. The motivation is to model the tip of a Magnetic Force Microscope, the separation between tip and sample playing the role of an impurity (a different hopping parameter). We study the level-spacing statistics of the whole system as a function of temperature down to 2 K. We find a large anomalous Hall effect (AHE) anisotropy in this system for $H \perp c$-axis, whereas the latter follows $\rho^2$ for $T < 150$ K. We tentatively interpret the behavior of $\rho_{xy}$ for $H \parallel c$-axis in terms of an intrinsic effect related to the inter-orbital hopping between degenerate $d$-orbitals. Such hopping is allowed for high symmetry points at the crystallographic dumb-bell sites in this configuration. On the other hand, there is no inter-orbital hopping for $H \perp c$-axis. However, a huge amplitude of the AHE resistivity for this configuration, which follows from skew scattering, is puzzling. Both the AHE anisotropy and the large skew scattering go away as more Fe is substituted by Co. We attribute this to variations in the electronic structure of the Y$_2$Fe$_{17-x}$Co$_x$ system when Co atoms start to occupy the dumb-bell crystallographic sites.

1:27PM B29.00012 Kondo decoherence: finding the right spin model for iron impurities in gold and silver, J. VON DELFT, Ludwig-Maximilians-University Munich, T.A. COSTI, L. BERGGVIST, Forschungszentrum Julich, A. WEICHSELBAUM, Ludwig Maximilians University Munich, T. MICKLITZ, A. ROSCH, University of Cologne, P. MAVROPOULOS, P. DEDERICHS, Forschungszentrum Julich, F. MALLETT, L. SAMINADAYAR, C. BÄUERLE, Institut Neel - CNRS and Universite Joseph Fourier — We exploit the decoherence of electrons due to magnetic dumb-bell sites in this configuration. On the other hand, there is no inter-orbital hopping for $H \perp c$-axis. However, a huge amplitude of the AHE resistivity for this configuration, which follows from skew scattering, is puzzling. Both the AHE anisotropy and the large skew scattering go away as more Fe is substituted by Co. We attribute this to variations in the electronic structure of the Y$_2$Fe$_{17-x}$Co$_x$ system when Co atoms start to occupy the dumb-bell crystallographic sites.

1:39PM B29.00013 Electronic Interactions between Au Films and the Prussian Blue Analog Co$_{3}[\text{Os}(\text{CN}_6)]_2^2$, T. WELLINGTON, Texas A&M University, Department of Physics, M. HILFIGER, Texas A&M University, Department of Chemistry, A. FORD, Texas A&M University, Department of Physics, C. AVENDANO, K. DUNBAR, Texas A&M University, Department of Chemistry, W. TEIZER, Texas A&M University, Department of Physics — The Prussian blue analog Co$_{3}[\text{Os}(\text{CN}_6)]$$_2$ exhibits photoinduced changes of magnetic behavior as well as charge transfer induced spin transitions at low temperature. Magnetic measurements on the bulk material show an increased magnetic susceptibility after illumination with red light, as the analog exhibits an abrupt spin transition due to enhanced cooperativity. We are exploring electronic interactions between this Prussian blue analog and gold films of varying thickness. Low-temperature measurements of the magnetoresistance of the gold films, with and without a surface layer of the analog, are performed. The study focuses on how the presence of the analog on the surface affects the transport properties within the gold film.

1:51PM B29.00014 ABSTRACT WITHDRAWN —
We have synthesized superlattices of (LaMnO$_3$)$_x$/(SrMnO$_3$)$_{1-x}$. The key experimental finding is that, below $T_N$, negative MR [defined as $(\rho(H)-\rho(0))/\rho(0)$ where $\rho$ is the electrical resistivity] is observed. Here we present evidence for the opposite behavior of MR in an intermetallic compound, viz., $\rho(H)/\rho(0)$ where $\rho$ is the electrical resistivity] is observed. Here we present evidence for the opposite behavior of MR in an intermetallic compound, viz., $\rho(H)/\rho(0)$. We observe a field-induced ferromagnetic transition in the magnetically ordered state ($T_N=69$ K). The key experimental finding is that, below $T_N$, $\rho$ is dramatically enhanced at all temperatures (resulting in large “positive” MR) at $H$, in sharp contrast to the expectation based on common knowledge. This finding bears significant relevance to electron scattering phenomena in general, and in particular in metamagnetic systems.

**Monday, March 16, 2009 11:15AM - 2:03PM**
Session B30 GMAG DMP: Focus Session: Manganite Superlattices 334

11:15AM B30.00001 Emergent properties of digital superlattices of LaMnO$_3$/SrMnO$_3$\(^1\), ANAND BHATTACHARYA, Center for Nanoscale Materials and Materials Science Division, Argonne National Laboratory — LaMnO$_3$ and SrMnO$_3$, both antiferromagnetic insulators, are end members of the La$_{1-x}$Sr$_x$MnO$_3$ phase diagram, which includes a highly spin-polarized ferromagnetic metal and a variety of orbital-ordered antiferromagnets. Interfaces between LaMnO$_3$ and SrMnO$_3$ provide a unique environment where the spin, charge and orbital degrees of freedom of each of the constituents may ‘reconstruct’, giving rise to collective states at interfaces that are qualitatively distinct from those in either LaMnO$_3$ or SrMnO$_3$. We have synthesized superlattices of (LaMnO$_3$)$_n$/(SrMnO$_3$)$_m$, where $n= q/(p+q)$, using ozone-assisted molecular beam epitaxy. Here, $p$ and $q$ represent integer layers of the constituents. These superlattices can be realized with interface roughness/intermixing limited to a region less than one unit-cell in extent. We will explore the properties of these ‘digital manganites’ for a range of $p/q$, including enhanced ordering temperatures compared to randomly alloyed samples, and provide experimental evidence for the interface reconstruction that is responsible for their emergent properties.

\(^1\)This work was supported by the US Department of Energy, Office of Basic Energy Sciences.

11:51AM B30.00002 Enhanced Antiferromagnetic Ordering Temperature in Metallic LaMnO$_3$/SrMnO$_3$ Superlattices , TIFFANY SANTOS, STEVEN MAY, ANAND BHATTACHARYA, Argonne National Lab, J. LEE ROBERTSON, Oak Ridge National Lab — The perovskite manganite La$_{1-x}$Sr$_x$MnO$_3$ has a rich magnetic phase diagram, exhibiting ferromagnetism (F) for La-rich compositions and antiferromagnetism (AF) for those that are Sr-rich. Our study focuses on the x=0.5 doping region containing the F-AF phase transition, particularly the role of strain and cation-site disorder in nucleating the F or AF state. Using ozone-assisted molecular beam epitaxy, we have prepared fully-epitaxial superlattices of LaMnO$_3$ and SrMnO$_3$ on SrTiO$_3$ substrates, along with random alloy films of La$_{1-x}$Sr$_x$MnO$_3$ with equivalent composition. In our digital synthesis method, whereby we interleave single unit-cell layers of undoped LaMnO$_3$ and SrMnO$_3$, we have eliminated disorder at the La/Sr cation site. Our structural characterization shows atomic layer precision in the synthesis of these superlattices. The structural, magnetic and transport properties of the superlattices are compared with those of the random alloys. A-type AF order (F alignment in-plane, AF alignment of adjacent planes) is verified by neutron diffraction, also revealing an enhanced Néel temperature with no F phase at higher temperature, in contrast to bulk. These AF thin films display metal-like behavior, opening the possibility of using the discrete layers of opposite spins for coherent spin transport. Supported by DOE, Office of Basic Energy Sciences.

12:03PM B30.00003 Theory of Manganite Superlattices\(^1\), ANDREW MILLIS, CHUNGWEI LIN, Department of Physics, Columbia University — A comprehensive theoretical treatment of (001) (LaMnO$_3$)$_n$/(SrMnO$_3$)$_m$ manganite superlattices is presented. The charge distribution, conductivity, and propagation through the superlattice of orbital and magnetic order are determined using dynamical mean field calculations in the superlattice geometry. General rules for predicting the behavior of manganite superlattices are outlined. Comparison is made to existing data and inconsistencies between theory and experiment are identified and discussed.

\(^1\)This research was supported by DOE ER-046196

12:15PM B30.00004 Control of Magnetism via Layer Thickness Modification in the LaMnO$_3$/SrMnO$_3$ Digital Superlattices and the Prediction of a Spin-Polarized 2DEG , BIRABAR NANDA, SASHI SATPATHY, University of Missouri-Columbia — We study the effect of layer thickness on the magnetic properties in the (LMO)$_{2n}$/SMO$_n$ superlattices using density-functional calculations. The change in the magnetic properties is shown to be controlled by the leakage of the Mn-$e_g$ electrons from the LMO layer to the SMO side. For $n=1$ superlattice, the weak potential barrier allows the Mn-$e_g$ electrons to spread across the entire superlattice, so that a uniform ferromagnetic behavior is obtained through carrier mediated Zener double exchange. For larger $n$, the strong potential barrier restricts the $e_g$ electron transfer to few layers adjacent to the interface, thus leaving the magnetism unchanged and bulk like away from the interface, while modifying the magnetism in the interfacial region. Finally, taking the example of a delta doped superlattice, (SMO)/(LMO)$_n$, we predict the formation of a spin-polarized two dimensional electron gas. The 2DEG, generated due to the confinement of the La ($d$) electrons in the direction normal to the interface, mediates a ferromagnetic alignment of the Mn-$e_g$ spins via double exchange which in turn spin polarizes the 2DEG.

\(^1\)Work supported by the US Department of Energy


12:27PM B30.00005 The onset of metallic behavior in strained (LaNiO$_3$)$_n$/(SrMnO$_3$)$_2$ superlattices , STEVEN MAY, Materials Science Division, Argonne National Laboratory, TIFFANY SANTOS, Center for Nanoscale Materials, Argonne National Laboratory, ANAND BHATTACHARYA, Center for Nanoscale Materials and Materials Science Division, Argonne National Laboratory — Motivated by predictions of collective ordering phenomena in LaNiO$_3$, we have grown strained (LaNiO$_3$)$_n$/(SrMnO$_3$)$_2$ superlattices on SrTiO$_3$ using ozone-assisted molecular beam epitaxy. The superlattices exhibit excellent crystallinity and interfacial roughness of less than one unit cell. The samples undergo a metal-insulator transition as $n$ is reduced from 4 to 2. Both $n = 1$ and 2 samples are insulating, however, they exhibit different transport behavior. The $n = 1$ sample acts as a gapped insulator, while the addition of a second LNO layer ($n = 2$) leads to hopping transport through non-gapped conduction channels. These results will be compared to (LaMnO$_3$)/(SrMnO$_3$) superlattices to highlight how interfacial charge transfer differs in the nickelate/manganite superlattices from their all-manganite counterparts. Supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.
12:39PM B30.00006 Electronic and crystal-field effects in the fine structure of electron energy-loss spectra of \( \text{La}_x \text{Ca}_{1-x} \text{MnO}_3 \). WEIDONG LUO, MARIA VARELA, JING TAO, STEPHEN J. PENNYCOOK, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The fine structure of oxygen K-edge electron energy-loss spectra (EELS) of transition-metal oxides is known to be correlated with nominal oxygen states (NOS) that are often interpreted as charge states. We report the results of a systematic study of O K-edge EELS fine structures in \( \text{La}_x \text{Ca}_{1-x} \text{MnO}_3 \) and their evolution as functions of doping \( x \). The calculated spectra, specifically the pre-peak intensities and peak separations, as functions of \( x \) are in excellent agreement with experimental data. The calculations show that the variation of the pre-peak's intensity with doping is controlled by the orbital occupancy of the majority-spin Mn 3d states while its width is controlled by crystal-field splitting. The energy separation between the pre-peak and the main peak also has a correlation with the doping parameter \( x \) and the NOS. The results confirm that the NOS extracted from EELS correlates with orbital occupancies but does not probe physical charges of the Mn sites. This research was sponsored in part by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering and by the McMinn Endowment at Vanderbilt University. Computations were performed at the National Energy Research Scientific Computing Center.

12:51PM B30.00007 Local Electronic Structure at Oxide-Oxide Interfaces Probed by Atomic Resolution Electron Energy Loss Spectroscopy \(^1\). AMISH SHAH, Dept. of Mat. Sci. Eng., Univ. of Illinois, Urbana-Champaign, Q. M. RAMASSE, National Center for Electron Microscopy, Lawrence-Berkeley National Laboratory, S. J. MAY, Materials Science Division, Argonne National Laboratory, J. G. WEN, Materials Res. Lab., Univ. of Illinois, Urbana-Champaign, J. N. ECKSTEIN, Dept. of Physics, Univ. of Illinois, Urbana-Champaign, A. BHATTACHARYA, Materials Science Division, Argonne National Laboratory, J.-M. ZUO, Dept. of Mat. Sci. Eng., Univ. of Illinois, Urbana-Champaign — We report an atomic resolution study of the electronic structure of 12 \( \times \) 4 \( \text{LaMnO}_3 \)-\( \text{SrMnO}_2 \) and 2 \( \times \) 2 \( \text{LaMnO}_3 \)-\( \text{SrTiO}_3 \) superlattices and their interfaces grown on \( \text{SrTiO}_3 \) by EELS. We correlated the interfacial electronic structure with the interfacial atomic structure using atomic resolution Z-contrast STEM using an electron probe of \( \geq 0.1 \) nm. The oxide superlattices were synthesized using molecular beam epitaxy. We measured the site-specific unoccupied states of oxygen atoms and transition metals. In the \( \text{MnO}-\text{SMO} \) system we found extra states (holes) near the Fermi level and their dependence on abruptness of interface. In \( \text{MnO}-\text{STO} \), we will present evidence of site-dependent electronic structure of oxygen and the Mn valence based on the L-edge ratios.

\(^1\)Supported by DOE BES

1:03PM B30.00008 Electronic properties of manganite / titanate superlattices \(^1\). MARIA VARELA, H. CHRISTEN, H. N. LEE, L. PETIT, T. SCHULTHESS, S. PENNYCOOK, Oak Ridge Natl. Lab., J. GARCÍA-BARRIOCANAL, A. RIVERA, F. Y. BRUNO, Z. SEFRIOUI, C. LEON, J. SANTAMARIA, Univ. Complutense, Spain — Here we report on the study of \( \text{LaMnO}_3 \)-\( \text{SrTiO}_3 \) interfaces. While \( \text{MnO} \) in bulk is an antiferromagnetic Mott insulator and \( \text{STO} \) is a band insulator, \( \text{MNO}/\text{STO} \) superlattices exhibit ferromagnetism and in some cases metallicty, both of which can be tuned by changing the layer thicknesses. We will compare the structure, chemistry and electronic properties of \( \text{MNO}/\text{STO} \) interfaces in high quality superlattices grown by pulsed laser deposition and high \( \text{O}_2 \) pressure sputtering. The distribution of defects and electronic properties will be studied through aberration corrected electron microscopy and electron energy loss spectroscopy. PLD superlattices show two alternating interface terminations, \( \text{LaO}-\text{TiO}_2 \) and \( \text{SrO}-\text{MnO}_2 \), which cause an asymmetry in the LMO layer electronic properties. Superlattices grown by sputtering show only one termination, \( \text{LaO}-\text{TiO}_2 \), giving an overall electron doping to the system. The role of interfacial charge transfer or localization, and any changes in electronic properties due to structural relaxations induced by epitaxial strain will be examined.

\(^1\)Research sponsored by US DOE and ORNL LDRD.

1:15PM B30.00009 Magnetic and structural phase transitions in epitaxial thin films of Manganites \(^1\). VALTERA LAUTER, HALEMARIAM AMBAYE, STEVEN NAGLER, HANS CHRISTEN, MIKE BIEGALSKI, Oak Ridge National Laboratory, SNS COLLABORATION, CNMS COLLABORATION — Understanding the magnetic properties of complex materials near interfaces is important for the development of functional nanostructures and devices. Epitaxial \( \text{LaMnO}_3 \) films were grown on \( \text{SrTiO}_3 \) substrates. Recent work on such thin-film samples has shown that “interface doping” can induce magnetism at interfaces. Our work on \( \text{LaMnO}_3 \)-\( \text{SrTiO}_3 \) interfaces has shown that the nature of the interface determines the magnetic structure - with the \( \text{MnO}_2 \)-\( \text{SrO} \) interface showing a different magnetization than the \( \text{LaO}-\text{TiO}_2 \) interface. To investigate these structures, we used polarized neutron reflectometry with off-specular scattering. Our results give evidence of reversible temperature- and field- dependent structural changes in \( \text{LaMnO}_3 \) film which undergo a phase transition. We determined that a structural phase transition in \( \text{SrTiO}_3 \) and the misfit strain trigger appearance of twins to reduce stresses and to adjust lattice mismatch between the film and the substrate. We show that a laterally correlated superstructure appear due to interaction of structural modifications with the magnetization the film.

\(^1\)This Research at Oak Ridge National Laboratory’s Spallation Neutron Source U. S. Department of Energy.

1:27PM B30.00010 Ferromagnetic Spin State of Manganite/SrTiO\(_3\) Interfaces in (110) Orientation . XINFEI LIU, JIANXING MA, TAO LIN, Department of Physics, University of California, Riverside, G. Y. GAO, W. B. WU, X. G. LI, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, JING SHI, Department of Physics, University of California, Riverside — The interface spin state of a ferromagnet (FM) can deviate significantly from its bulk spin state and this effect could be strongly orientation-dependent especially in manganites. We have successfully fabricated high-quality (110)-oriented [\( \text{La}_{0.5} \text{Sr}_{0.5} \text{MnO}_3 \) (t) / \( \text{SrTiO}_3 \) (3ML)], superlattices (t ranging from 3 to 15 ML), which are characterized by the atomic force microscopy, high-resolution transmission electron microscopy, x-ray diffraction and magnetometry. Compared to (100)-oriented counterparts, LSMO in (110)-oriented superlattices has a thinner deadlayer at LSMO/STO interface. From the thickness (t) dependence of the superlattice magnetic moment, we extract the interface contribution and find that the interface moment is close to that of the bulk, suggesting that the (110)-oriented interface adsorb a FM spin ground state. This differs significantly from the spin canting state at (100)-oriented LSMO/STO interface that was previously reported by other groups. Our results indicate that the magnetism of manganese interface may be manipulated by taking advantage of the orientation-dependent nature of the exchange interactions.

1:39PM B30.00011 Enhanced Low Field Magnetoresistance in \( \text{La}_{0.67} \text{Ca}_{0.33} \text{MnO}_3 / \text{La}_{0.5} \text{Ca}_{0.5} \text{MnO}_3 \) superlattices . P.V. WADECAR, Q.Y. CHEN, O. LOZANO, P.V. CHINTA, W.K. CHU, D. WIJESUNDERA, A. Department of Physics & Texas Center for Superconductivity, University of Houston, Texas 77024, USA, C.S. LIN, P.H. TSENG, Y.T. LIN, L.W. TU, C.P. LIN, H. CHOLI, C.C. KUO, Department of Physics & Center for Nanoscience and Nanotechnology, National Sun Yat Sen University, Kaohsiung, Taiwan, Republic of China, N.J. HO, Department of Materials and Optoelectronic Sciences and Technology, National Chiao Tung University, Hsinchu, Taiwan, National Science Council, National Sun Yat-Sen University, Kaohsiung, Taiwan, H.W. SEO, Department of Physics, University of Arkansas, Little Rock, AR 72204 — We have grown \([ \text{La}_{1-x} \text{Ca}_x \text{MnO}_3 ](x=0.33) \) serves as the ferromagnetic layer while \( \text{La}_{1-x} \text{Ca}_x \text{MnO}_3 (x=0.5) \) serves as the spacer layer on \( \text{LaAlO}_3 \) substrates by magnetron sputtering. The samples were characterized by XRD, Magneteto-transport measurements, Rutherford backscattering spectrometry, and atomic force microscopy. Enhanced longitudinal magnetoresistance (MR) under an applied field B, defined as \( \text{MR} (B) = (\rho(B))/\rho(0) - 1 \), was as much as -49% at \( B=0.5 \) Tesla and \( T=90 \) K. The causes for this enhancement not seen at low field in other single-layered films of \( x=0.33 \) and the correlation of oxygen annealing with the MR effects for the superlattices will be presented.
11:15AM B31.00001 Multiple magnetic phases in the frustrated S=1 spin-dimer compound Ba₃Mn₂O₅₁⁺. ERIC SAMULON, Stanford University — Ba₃Mn₂O₅ is a spin-dimer compound based on pairs of S=1/2 Mn²⁺ ions arranged on a triangular lattice. Antiferromagnetic intradimer exchange leads to a singlet ground state in zero-field. Interactions between dimers broaden the triplet and quintuplet bands such that application of a magnetic field leads to multiple states marked by long range order above characteristic critical fields. Here we present results of magnetization, heat capacity, magnetocaloric effect and torque magnetometry measurements of single crystal samples which reveal a complex phase diagram containing at least three distinct ordered states across the triplet and quintuplet regimes. Much of the phase diagram can be understood in terms of an effective spin 1/2 Hamiltonian containing only the lowest energy states (|0,0⟩ & |1,1⟩ and |1,1⟩ & |2,2⟩, referred to the dimer states, for the sinlet-triplet and triplet-quintuplet regimes respectively). Two distinct ordered states are observed in the sinlet-triplet regime, which can be ascribed to the delicate interplay between single spin anisotropy and antiferromagnetic interdimer exchange on the frustrated triangular lattice.

11:15AM B31.00002 Frustrated magnetism in the diamond-chain like compound Ba₃Cu₃Sc₂O₁₂. A.V. MAHAJAN, Department of Physics, IIT Bombay, B. KOTESWARA RAO, Dept. of Physics, IIT Bombay, B. BOBROFF, Labo. de Physique des Solides, Orsay, France — The structure of Ba₃Cu₃Sc₂O₁₂, having chains of corner-shared square plaquettes, is reminiscent of the “diamond chain” compound Cu₃(CO₃)₂(OH)₂ which has shown novel magnetic properties. We report preparation of polycrystalline samples of Ba₃Cu₃Sc₂O₁₂ followed by temperature dependent magnetic susceptibility χ(T) and heat capacity C_p(T) measurements in applied magnetic fields up to H = 90 kOe. At high-T, χ(T) is fitted by the Curie-Weiss law (χ(T) = C/(T-θ)) and is suggestive of ferromagnetic interactions (θCW ~ 70 K). However, in low-fields, the χ(T) shows a sharp peak at TN ~ 16 K and the variation at lower temperatures is indicative of antiferromagnetic ordering. Clear evidence of the transition at TN is also seen in heat capacity data. The sharp peak in χ(T) and C_p(T) moves to lower temperatures with increasing H. The TN is found to be strongly lowered by an applied field and TN ~ 0 for H ~ 70 kOe. Further work to understand the relative exchange couplings between various Cu atoms is currently in progress.

12:03PM B31.00003 NMR Response in Antiferromagnetic Spin-1/2 Chains. JESKO SIRKER, Max-Planck Institute for Solid State Research, NICOLAS LAFLORENCIE, CNRS - LPS Orsay — Non-magnetic impurities break a quantum spin chain into finite segments and induce Friedel-like oscillations in the local susceptibility near the edges. The signature of these oscillations has been observed in Knight shift experiments on the high-temperature superconductor YBa₂Cu₃O₇ and on the spin-chain compound Sr₂CuO₃. Here we analytically calculate NMR spectra, compare with the experimental data, and give a simple criterion to determine the impurity concentration. Our results are based on a parameter-free formula for the local susceptibility of a finite spin chain obtained by bosonization which is checked by comparing with quantum Monte Carlo calculations.

12:15PM B31.00004 Controlling Luttinger Liquid Physics in Spin Ladders under Magnetic Field. C. BERTHERT, M. KLJANŠEK, M. HORVATIĆ, GHMF, CNRS, F-38042 Grenoble Cedex 09, France, H. MAYAFFRE, LSP Orsay — Non-magnetic impurities break a quantum spin chain into finite segments and induce Friedel-like oscillations in the local susceptibility near the edges. The signature of these oscillations has been observed in Knight shift experiments on the high-temperature superconductor YBa₂Cu₃O₇ and on the spin-chain compound Sr₂CuO₃. Here we analytically calculate NMR spectra, compare with the experimental data, and give a simple criterion to determine the impurity concentration. Our results are based on a parameter-free formula for the local susceptibility of a finite spin chain obtained by bosonization which is checked by comparing with quantum Monte Carlo calculations.
12:39PM B31.00006 Spin order of the classical Kagome antiferromagnet: via effective Hamiltonians . CHRISTOPHER L. HENLEY, Cornell Univ. — The classical Heisenberg Kagomé-lattice antiferromagnet (KAF) is only known to have a coplanar “spin nematic” (or octupole) order, so that low-energy states are labeled by colors. Contrary to accepted phenomenology,1 I propose that these colorings develop long-range order,2 first, from the spin-wave Hamiltonian up to 4th order, most modes are integrated out, leaving an effective quartic Hamiltonian $Q$ for just the “soft” (zero at harmonic order) modes. Writing it $Q = Q_0 + Q'$, where only $Q'$ depends on the discrete coplanar state, $Q'$ is treated as a perturbation, and its expectation in the $Q_0$ ensemble becomes an effective Hamiltonian $\Phi$ for the colorings. The couplings in $\Phi$ are estimated using “Coulomb phase” coarse-grainings.2 Following Huse & Rutenberg,3 I observe the unweighted coloring model sits at a roughening transition, hence $\Phi$ drives the KAF to long-range order of the $\sqrt{3} \times \sqrt{3}$ type (modulus the inevitable gradual orientation fluctuations of the spin plane). A similar effective Hamiltonian exists for related $d = 3$ lattices, but cannot produce order.

2 C. L. Henley, arxiv:0811.0026.

12:51PM B31.00007 Quantum stabilization of 1/3 magnetization plateau in $\text{Cs}_2\text{CuCl}_4$. OLEG STARYKH, University of Utah, JASON ALICEA, California Institute of Technology, ANDREY CHUBUKOV, University of Wisconsin — We consider the phase diagram of a spatially anisotropic 2D triangular antiferromagnet in a magnetic field. Classically, the ground state is umbrella-like for all fields, but we show that the quantum phase diagram is much richer and contains a 1/3 magnetization plateau, two commensurate planar states, two incommensurate chiral umbrella phases, and, possibly, a spin density wave state separating the two chiral phases. Our analysis sheds light on several recent experimental findings for the spin-1/2 system $\text{Cs}_2\text{CuCl}_4$.

1:03PM B31.00008 Magnetic properties of bilayer triangular lattice1, FEI-MING HU, SHI-QUAN SU, TIAN-XING MA, HAI-QING LIN, Department of Physics and the Institute of Theoretical Physics, the Chinese University of Hong Kong — We study magnetic properties of the single-band Hubbard model on a coupled bilayer triangular lattice by using the determinant quantum Monte Carlo method. Simulations are focused in the region near the van Hove singularities. We perform investigations on two kinds of double layer triangular lattices, one is a simple triangular lattice which has only one nearest neighbor between two layers for every atom and another one is a graphene-like structure which has three nearest neighbors between two layers for every atom. We compare their magnetic properties in the view of the itinerant electron ferromagnetic theory of attribute their behaviors to the density of states on the Fermi surface.

1This work is supported by HK RGC Grant 402107

1:15PM B31.00009 Dzyaloshinskii-Moriya interactions in valence bond systems 1, KIRILL SHTENGEL, KUMAR RAMAN, MAYAR TOVAR, UC Riverside — We investigate the effect of Dzyaloshinskii-Moriya interactions on the low temperature magnetic susceptibility for a system whose low energy physics is dominated by short-range valence bonds (singlets). Our general perturbative approach is applied to specific models expected to be in this class, including the Shastry-Sutherland model of the spin-dimer compound $\text{SrCu}_2(\text{BO}_3)_2$ and the antiferromagnetic Heisenberg model of the recently discovered $S = 1/2$ kagome compound $\text{ZnCu}_2(\text{OH})_6\text{Cl}_2$. The central result is a short-ranged valence bond phase, when perturbed with Dzyaloshinskii-Moriya interactions, will remain time-reversal symmetric in the absence of a magnetic field but the susceptibility will be nonzero in the zero temperature limit. Applied to $\text{ZnCu}_2(\text{OH})_6\text{Cl}_2$, this model provides an avenue for reconciling experimental results, such as the lack of magnetic order and lack of any sign of a spin gap, with known theoretical facts about the kagome Heisenberg antiferromagnet.

1NSF DMR-0748925

1:27PM B31.00010 Hierarchical mean-field approach to the $J_1-J_2$ Heisenberg model on a square lattice . LEONID ISAEV, GERARDO ORTIZ, Indiana University, Bloomington IN, USA, JORGE DUKELSKY, Instituto de Estructura de la Materia - CSIC, Madrid, Spain — We study the quantum phase diagram and excitation spectrum of the frustrated $J_1-J_2$ spin-1/2 Heisenberg Hamiltonian. A hierarchical mean-field approach, at the heart of which lies the idea of identifying relevant degrees of freedom, is developed. Thus, by performing educated, manifestly symmetry preserving mean-field approximations, we unveil fundamental properties of the system. We then compare various coverings of the square lattice with plaquettes, dimers and other degrees of freedom, and show that only the symmetric plaquette covering, which reproduces the original Bravais lattice, leads to the known phase diagram. The intermediate quantum paramagnetic phase is shown to be a (singlet) plaquette crystal, connected with the neighbouring Néel phase by a continuous phase transition. We also introduce fluctuations around the hierarchical mean-field solutions, and demonstrate that in the paramagnetic phase the ground and first excited states are separated by a finite gap, which closes in the Néel and columnar phases. Our results suggest that the quantum phase transition between Néel and paramagnetic phases can be properly described within the Ginzburg-Landau-Wilson paradigm.

1:39PM B31.00011 Mixed exchange antiferromagnetic/ferromagnetic $S=1/2$ Heisenberg rectangular lattices , BRIAN KEITH, TOM VALLEAU, FAN XIAO, MARK TURNBULL, CHRIS LANDEE, Clark University, LANDEE/TURNBULL MAGNET LAB TEAM — The susceptibilities of mixed antiferromagnetic/ferromagnetic rectangular Heisenberg lattices of $S = 1/2$ have been simulated using Quantum Monte Carlo techniques. These simulations include lattices in which the stronger interaction is ferromagnetic or antiferromagnetic along with the isotropically mixed lattice, which has two exchange strengths, $J$ and $J'$, are related by $J' = \alpha J$, where $\alpha$ is the aspect ratio which ranges from $0 \leq \alpha \leq 1$. These simulations were done for $0 < \alpha < 1$ in 0.05 increments. The results are discussed and the models are used to fit suspected mixed antiferromagnetic/ferromagnetic rectangulars such as $\text{Cu}_2(\text{pyz})_2(\text{NO}_3)_2(\text{HCO}_2)$ and $\text{Cu}_2(\text{pyz})_2(\text{N}_2)$.

1:51PM B31.00012 ABSTRACT WITHDRAWN —

2:03PM B31.00013 $\text{Ce}_2\text{Pt}_2\text{Pb}$ : Frustrated heavy fermion system with the Shasry-Sutherland lattice . MOO SUNG KIM, Brookhaven National Laboratory. MEIGAN ARONSON, Brookhaven National Laboratory, Stony Brook University — We have synthesized single crystals of $\text{Ce}_2\text{Pt}_2\text{Pb}$ which has the Shasry-Sutherland lattice network of Ce ions on the crystallographic c-plane, that can induce magnetic frustration. The specific heat, magnetic susceptibility, and resistivity were measured for as-grown crystals. Above 30 K, Curie-Weiss behavior is found in the magnetic susceptibility, with a Ce moment of 2.33 $\mu_B$/Ce and a Weiss temperature of -15 K, indicating antiferromagnetic interactions among the Ce$^{3+}$ ions. The magnetic specific heat rises from a minimum at 15 K to a broad maximum at 2 K, before falling to a heavy fermion value of $\sim 0.8$ J/Ce-mol K$^2$ at the lowest temperature. The entropy reaches only 1/2Rln2 at the maximum in the specific heat, and the full double ground state Rln2 is only recovered at 15 K. $\text{Ce}_2\text{Pt}_2\text{Pb}$ is an unusual material, in which a heavy fermion liquid with short range antiferromagnetic order emerges from a strongly frustrated and fluctuating paramagnetic state.
The sound attenuation displays a double peak structure and looks like an almost exact copy of the corresponding curves, characterizing behavior of profound rounded dips at temperature $T_c$. Neutron scattering measurements of the magnetic excitations in the $S=1/2$ antiferromagnet La$_2$CuO$_4$ reveal profound rounded dips at the phase transition [1,2]. We observe collective spin-excitations from the full first Brillouin-zone, in contrast to Inelastic Neutron Scattering [4]. At the $Q$ edge site-sensitive hole-excitation studies of the chain- and ladder-subsystems were performed, giving insight into the character of the holes. [1] T. Vuletic et al., Physics Reports 428, 169-258 (2006). [2] A. Kotani and K. Satow, H. Takagi (Tokyo), J.D. Denlinger (ALS). This suggests the embedding of dilute impurities as a powerful mean to probe weak and, possibly, spatially inhomogeneous order in solid-state systems. In particular, the intensity of the spin wave pole deviates strongly from that predicted by SW theory near the $Q$ edge site-sensitive hole-excitation studies of the chain- and ladder-subsystems were performed, giving insight into the character of the holes. [1] T. Vuletic et al., Physics Reports 428, 169-258 (2006). [2] A. Kotani and K. Satow, H. Takagi (Tokyo), J.D. Denlinger (ALS).
is supported by US Dept. of Energy at MU.

nm and thicknesses of 40 nm, coupled via permalloy bridges of width ranging from 0 to 60 nm, were fabricated using e-beam lithography. In the perpendicularly

Spin wave spectra in exchange coupled nanoscale dot chain arrays were studied using ferromagnetic resonance. The dot chain arrays, with dot diameters of 300

of Physics, Miami University, LIESL FOLKS, JORDAN A. KATINE, MATTHEW J. CAREY, San Jose Research Center, Hitachi Global Storage Technologies —

is recorded via longitudinal Kerr-magnetometry. The relaxation data are analyzed by scaling plots revealing universal aspects of aging. Financial support by

is discussed in terms of the interplay between magnetism and orbital order.

electrons. The nature of the orbital order in these vanadites has been a matter of significant controversy, particularly with respect to whether the different

orbital-ordered phases of YVO_{3} and LaVO_{3} are best described by a novel orbital-Peierls model or more traditional Jahn-Teller interactions. Here we report on a neutron scattering study of the magnetic correlations in Y_{0.7}La_{0.3}VO_{3}, which may be expected to depend sensitively on the orbital degrees of freedom. The results are discussed in terms of the interplay between magnetism and orbital order.

This work is supported by USDOE(DE-FG02-03ER46064) in Buffalo, by RC CCSA #7669 in Fresno, and by USDOE(DE-FG02-04ER46105) and

This work is supported by NSF(DMR0820478) in San Diego.

12:39PM B32.00008 Neutrons Scattering Study of Magnetic Correlations in Y_{0.7}La_{0.3}VO_{3} \textsuperscript{1}. SUNG CHANG, NIST Center for Neutron Research, JIAQIANG YAN, Ames Laboratory, ROBERT MCQUEENEY, Iowa State University — RVO_{3} (R = rare earth) perovskite vanadites exhibit multiple orbital and spin orderings and provide a unique opportunity to study the spin-orbital-lattice coupling of \tau electrons. The nature of the orbital order in these vanadites has been a matter of significant controversy, particularly with respect to whether the different orbital-ordered phases of YVO_{3} and LaVO_{3} are best described by a novel orbital-Peierls model or more traditional Jahn-Teller interactions. Here we report on a neutron scattering study of the magnetic correlations in Y_{0.7}La_{0.3}VO_{3}, which may be expected to depend sensitively on the orbital degrees of freedom. The results are discussed in terms of the interplay between magnetism and orbital order.

1This work utilized facilities supported in part by the National Science Foundation under Agreement No. DMR-0454672.

12:51PM B32.00009 ABSTRACT WITHDRAWN –

1:03PM B32.00010 Possible Observation of Electromagnons in BiFeO_{3} Crystal , PAULINE ROVILLAIN, YANN GALLAIS, ALAIN SACUTO, Laboratoire Matériaux et Phénomènes Quantiques Université Paris 7, France, RICARDO LOBO, ESPCI, DOROTHÉE COLSON, DELPHINE LEBEUGELE, CEASPEC, ROGERIO DE SOUSA — We show the first optical observation via inelastic light scattering of sharp low energy modes in multiferroic BiFeO_{3}. We have detected two different modes (\Psi and \Phi modes) and interpreted them as the optical fingerprint of the cycloidal magnetic order. The energies of the \Phi modes are equally spaced and exhibit a linear dependence as a function of the mode index (n) down to zero while the energy sequence of the \Psi modes is not equally spaced and exhibit a gap at low energy. Our experimental data are in remarkable agreement with the theory of de Sousa and Moore who pointed out that these modes could possibly be observed due to coupling between spins and lattice degrees of freedom. These experimental findings offer a unique opportunity for optical probing of the electromagnetic excitations of multiferroics. [1] Cazayous et al., Phys. Rev. Lett. 101, 097003 (2008).

1:15PM B32.00011 Magnon Sidebands and Spin-Charge Coupling in Bismuth Ferrite Probed by Nonlinear Optical Spectroscopy , AMIT KUMAR, M. RAMIREZ, S. DENEV, N. PODRAZA, X. XI, R. RAI, Y-H. CHU, J. SEIDEL, L. MARTIN, J. IHLEFELD, J. KLUG, M. BEDZYK, O. AUCIELLO, D. SCHLOM, R. RAMESH, J. ORENSTEIN, J. MUSFELDT, V. GOPALAN — The interplay between spin waves (magnons) and electronic structure in materials leads to the creation of additional bands associated with electronic energy levels, called magnon sidebands which are difficult to probe due to their smaller energy scales (meV). Linear light absorption and scattering techniques at low temperatures are traditionally used to probe these electronic sidebands. We show that optical second harmonic generation (SHG) can successfully probe the magnon sidebands at room temperature and up to 723K in bismuth ferrite, associated with large wave-vector multi-magnon excitations which linear absorption studies have thus far been unable to resolve. Polarized light studies and the temperature dependence of these sidebands reveal a spin-charge coupling interaction between the spontaneous polarization (P_s) and antiferromagnetic order parameter, L in bismuth ferrite, that persists with short range correlation well into the paramagnetic phase.

1:27PM B32.00012 Aging in Co/Cr Superlattices , T. MUKHERJEE, University of Nebraska-Lincoln, M. PLEIMLING, Virginia Polytechnic Institute and State University, CH. BINEK, University of Nebraska-Lincoln — Aging phenomena are observed in various systems brought into non-equilibrium and subsequently showing slow relaxation dynamics. Magnetic specimens with well defined interactions and dimensions can serve as model systems for universal aspects of aging. Magnetic thin films provide access to a wide range of microscopic parameters. Superlattice structures allow tuning the intra and inter-plane exchange and enable geometrical confinement of the spin fluctuations. We use Co/Cr thin film superlattices to study magnetic aging. The static and dynamic properties are affected via the Co and Cr film thicknesses. T_C of the Co films is reduced from the bulk value by geometrical confinement. Non-ergodic behavior sets in at a tunable temperature T^* in a range of some 100K above zero. Cr provides antiferromagnetic coupling between the Co films. Non-equilibrium spin states are set via low field cooling in 5mT in-plane magnetic field to below T^*. Next various in-plane magnetic set fields of some 10-100 mT are applied and the sample is exposed to the latter for various waiting times t_w, respectively. After removing the field, relaxation of the magnetization is recorded via longitudinal Kerr-magnetometry. The relaxation data are analyzed by scaling plots revealing universal aspects of aging. Financial support by Teledyne-Isco, NRI, and NSF through EPSCOR, Career DMR-0547887, and MRSEC.

1:39PM B32.00013 Exchange-coupling modified spin wave spectra in the perpendicularly magnetized permalloy nanodot chain arrays , JIAN DOU, SARAH C. HERNANDEZ, CHENGTAO YU, MICHAEL J. PECCHAN, Department of Physics, Miami University, LIESL FOLKS, JORDAN A. KATINE, MATTHEW J. CAREY, San Jose Research Center, Hitachi Global Storage Technologies — Spin wave spectra in exchange coupled nanoscale dot chain arrays were studied using ferromagnetic resonance. The dot chain arrays, with dot diameters of 300 nm and thicknesses of 40 nm, coupled via permalloy bridges of width ranging from 0 to 60 nm, were fabricated using e-beam lithography. In the perpendicularly magnetized isolated dots, multiple sharp ferromagnetic resonant peaks were observed which is associated with the quantized in-plane wave vector due to the finite dot radius. These spectrum lines shift to higher fields for samples with wider bridges due to the increasing effective demagnetizing factor. Additional higher order spin wave modes were observed as satellite peaks near the resonance peaks at both higher and lower fields, with larger separation between adjacent spin wave peaks for wider bridge samples. These extra spin wave modes, associated with the inter-dot exchange coupling, will be described in detail. This work is supported by US Dept. of Energy at MU.

11:15AM B33.00001 Making superconducting transition temperature higher in Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$ $^3$ XIAO-JIA CHEN, VIKTOR V. STRUZHVIN, RUSSELL J. HEMLEY, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, YONG YU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, CHENG-TIAN LIN, Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — We report an experimental finding of $T_c$ enhancement in optimally doped Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10+\delta}$. We found that the generally observed pressure effect on $T_c$, i.e., $T_c$ first increases with pressure and then decreases after passing a maximum at an optimal pressure, is only held below a critical pressure around 24 GPa in this multilayer material. After that $T_c$ enhances remarkably upon further compression, considerably surpassing the first maximum. The critical pressure was then considered as the crossover from antiferromagnetism to superconductivity in the inner Cu$_2$O plane. The afterwards $T_c$ enhancement was suggested to be through the optimization of two competing energy scales (pairing and phase ordering) of different CuO$_2$ planes. The results have important implications for engineering superconductors with much higher $T_c$’s at ambient conditions.

$^3$This work was supported by the DOE, CDAC and NSFC.

11:27AM B33.00002 Specific heat of underdoped high $T_c$ superconductors from phenomenological models. J. P. F. LEBLANC, E. J. NICOL, University of Guelph, J. P. CARBOTTE, McMaster University — Inspired by phenomenological models for the pseudogap state, for example, the model of Yang, Rice and Zhang[1], we have calculated the specific heat for the underdoped cuprate superconductors. Results will be shown for both the pseudogap and superconducting state as a function of doping. Comparison between models and with experiment will be made. [1] K.Y. Yang, T.M. Rice and F.C. Zhang. Phys. Rev. B 73, 175411 (2006).

11:39AM B33.00003 Resistive switching in YBa$_2$Cu$_3$O$_{7-\delta}$ CARLOS ACHA$^1$, MARCELLO J. ROZENBERG$^2$, Departmento de Fisica - FCEyN - Universidad de Buenos Aires — We report on the nonvolatile and polarity dependent resistance switching of metal- YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) ceramic superconductor interfaces that also extends macroscopically to the bulk YBCO. We show that electric pulses mainly modify the connectivity of the ceramic grains of the bulk material, affecting the geometrical conducting factor near the interface and controlling the superconducting percolating path in the bulk. Relaxation processes of the resistivity after applying the pulses, not associated with heating effects, are also observed. We also report on the temperature sensitivity of the resistivity switches in the bulk, which also depend on the conditions of both high and low resistance states and the voltage needed to produce the switching decrease with increasing temperature. The origin of this switching effect may be related to electric field-induced oxygen ion migration, which modifies the oxygen content at grain boundaries and controls the electric transport of ceramic superconductors.

$^1$member of CONICET and of the Asociacion Fisica Argentina
$^2$also at Laboratoire de Physique des Solides, CNRS-Universite de Paris-Sud, Orsay, France

11:51AM B33.00004 Calculation of diffusion coefficient in Au diffusion-doped Bi$_{1.8}$Pb$_{0.25}$Sr$_{1.9}$Ca$_{2.1}$Cu$_3$O$_y$ by EDXRF measurements$^1$, MUSTAFA AKDOGAN, Abant Izzet Baysal University, OZGUR OZTURK, Kastamonu University, UGUR CEVIK, Karadeniz Technical University, AHMET VARIILCI, CABIR TERZIOGLU, Abant Izzet Baysal University — Gold (Au) diffusion in superconducting Bi$_{1.8}$Pb$_{0.25}$Sr$_{1.9}$Ca$_{2.1}$Cu$_3$O$_y$ was investigated over the temperature range 500-800 $^\circ$C by the EDXRF technique. It is found that the Au diffusion coefficient decreases as the diffusion-annealing temperature decreases. The temperature dependences of Au diffusion coefficient in grains and over boundaries are described by the relations $D_1=6.7	imes10^{-5}\exp(-1.19E/k_BT)$ and $D_2=9.7	imes10^{-6}\exp(-1.09E/k_BT)$, respectively. The diffusion doping of Bi-2223 by Au causes a significant increase of the lattice parameter c by about 0.19%. For the Au-diffused samples, transport measurements indicated the $T_c$ increased from 100 to 104K and the J$_c$ increased from 40 to 125Acm$^{-2}$, in comparison with those of undoped samples. From SEM and XRD measurements it is observed that the Au doping of the sample improved the surface morphology and increased the ratio of the high-$T_c$ phase to the low-$T_c$ phase. The possible reasons for the observed improvement due to Au diffusion are also discussed.

$^1$This work supported by TUBITAK under grant contract No: 104T323 and 104T325.

12:03PM B33.00005 Charge distribution on planar oxygens in an underdoped High-$T_c$ cuprate: La(2-$x$)Sr($x$)CuO(4) via $^{17}$O NMR. GREG BOEBINGER, ROBERT SMITH, ARNEIL REYES, PHILIP KUHNS, NNMFL/FSU, TAKASHI IMAI, McMaster University/CIFAR, P. M. SINGER, Schlumberger-Doll Research Center, E. CHOU, National Taiwan University, K. HIROTA, University of Tokyo — Our recent studies revealed that the post-annealing to control cation composition largely changes superconducting properties of cuprate superconductors, such as Bi-based compounds and the RE123 system. For example, the $T_c$ of Bi(Ph)2223 was enhanced up to 118 K by post-annealing at ~950 K in air, while it was a typical value of 110 K before post-annealing. Strong correlation between the $c$-axis length and $T_c$ suggested that cation composition plays a crucial role to determine superconducting properties of this compound. On the other hand, substitution of RE for Ba-site in RE123 has been well recognized for light-RE123. However, such RE-rich RE123 compounds were found to form even for heavy-RE123 including Y123, which has been considered as a compound free from cation nonstoichiometry. The Y-rich Y123 exhibited suppressed $T_c$ down to ~80 K and apparently short $c$-axis length. These result indicated that intrinsic physical properties of layered cuprates should be reexamined after careful control of cation stoichiometry besides control of cation composition, because nonstoichiometric cation composition and its local fluctuation strongly affect electronic and vortex systems and related flux pinning properties.

12:15PM B33.00006 Magnetic Breakdown in the Cuprates, JEAN-MICHEL CARTER, DANIEL PODOLSKY, HAE-YOUNG KEE, University of Toronto — Following the recent observations of quantum oscillations in YBa$_2$Cu$_3$O$_{6.5}$ materials, we study different Fermi surface topologies in order to make a prediction on the nature of the topology of said Fermi surfaces in the cuprates.

12:27PM B33.00007 Important issues from uncontrolled cation nonstoichiometry in well-known cuprates, JUN-ICHI SHIMOYAMA, HIRAKU OGINO, SHIGERU HORII, YUHYA YAMAZAKI, KOICHI KAKU, YUI ISHII, KOHJI KISHIO, University of Tokyo — Our recent studies revealed that the post-annealing to control cation composition largely changes superconducting properties of cuprate superconductors, such as Bi-based compounds and the RE123 system. For example, the $T_c$ of Bi(Ph)2223 was enhanced up to 118 K by post-annealing at ~950 K in air, while it was a typical value of 110 K before post-annealing. Strong correlation between the $c$-axis length and $T_c$ suggested that cation composition plays a crucial role to determine superconducting properties of this compound. On the other hand, substitution of RE for Ba-site in RE123 has been well recognized for light-RE123. However, such RE-rich RE123 compounds were found to form even for heavy-RE123 including Y123, which has been considered as a compound free from cation nonstoichiometry. The Y-rich Y123 exhibited suppressed $T_c$ down to ~80 K and apparently short $c$-axis length. These result indicated that intrinsic physical properties of layered cuprates should be reexamined after careful control of cation stoichiometry besides control of cation composition, because nonstoichiometric cation composition and its local fluctuation strongly affect electronic and vortex systems and related flux pinning properties.
Applications, including operation as a fast, localized helium thermometer and as a transducer in superfluid hydrodynamic experiments, will be discussed.

The sample is a thin film with a large elastic free path (11 µm) deposited on a silicon oxide wafer. It is shown that PNR can resolve the difference between the reflected neutron spin asymmetries predicted by the local and nonlocal theories of superconductivity and therefore can be used for direct measurements of the microscopic intrinsic parameters of superconductors. The experimental data support the nonlocal theory, which predicts a nonmonotonic decay of the magnetic field.

12:39PM B33.00008 Evidence for nonmonotonic magnetic field penetration in a Pippard superconductor

NIKLAS KOSHEVNIKOV, Tulia Community College, CLAUDIU GIURANU, University of Lille, MARGRIET VAN BAEL, KRISTA TEMST, CHRIS VAN HAESENDONCK, Katholieke Universiteit Leuven, TODD MISHONOVA, Sr. Clement of Ohrad University at Sofia, TIMOTHY CHARLTON, ROBERT DALGIES, Rutherford Appleton Laboratory, YURI KHAIKOV, YURI NIKITENKO, VICTOR AKSENOV. Joint Institute for Nuclear Research, VLADIMIR GLADILIN, Katholieke Universiteit Leuven, VLADIMIR FOMIN, JOZEF DEVREESE, Universiteit Antwerpen, JOSEP INDEKEU, Katholieke Universiteit Leuven — Polarized neutron reflectometry (PNR) provides evidence that nonlocal electrolydronics governs the magnetic field penetration in an extreme low-τ superconductor. The sample is a thin film with a large elastic free path (11 µm) deposited on a silicon oxide wafer. It is shown that PNR can resolve the difference between the reflected neutron spin asymmetries predicted by the local and nonlocal theories of superconductivity and therefore can be used for direct measurements of the microscopic intrinsic parameters of superconductors. The experimental data support the nonlocal theory, which predicts a nonmonotonic decay of the magnetic field.

12:51PM B33.00009 ABSTRACT WITHDRAWN —

1:03PM B33.00010 Engineering Thin Film Superconductivity toward Single Quantum Channel Limit

SHENGYONG QIN, JUNGDAM KIM, QIAN NIU, CHIH-KANG SHIH, University of Texas at Austin — Traditional studies of two-dimensional superconductors were limited to the regime where the superconducting order parameter behaves as a two-dimensional wave function but the underline electrons are still three dimensional. Recent advancement of materials synthesis has enabled one to grow epitaxial thin superconductor thin films (e.g. Pb) on semiconductor substrates (e.g. Si or Ge) with unprecedented control in crystallinity, atomic smoothness and the layer thickness, thus opening up new opportunities in investigations of two-dimensional superconductivities. Indeed, quantum oscillations of the superconducting order parameter as a function of film thickness have been observed. Moreover, it was found that superconductivity remains very robustness even for films as thin as 5 ML. An interesting question arises as to what extent the robustness of superconductivity remains in even thinner regime. This work presents the case of thin film superconductivity in extreme confinement limit when only one quantum channel is present (i.e. when k_FL = π).

1:15PM B33.00011 Competition between pairing and magnetic interactions

RAIMUNDO DOS SANTOS, PEDRO BERTUSSI, Universidade Federal do Rio de Janeiro, ANDRE MALVEZZI, Universidade Estadual Paulista, THEREZA PAIVA, Universidade Federal do Rio de Janeiro — We discuss the interplay between pairing and magnetism by considering a model system composed of both tight-binding electrons and localized moments; the conduction electrons tend to form Cooper pairs due to a local (on-site) attractive interaction, U, while they also have a Kondo-like coupling, J, with the local moments. Density matrix renormalization group diagonalization on finite one-dimensional lattices (up to 60 sites) is used to calculate magnetic and pairing correlation functions, as well as structure factors in the ground state, in the case of electron density 1/3. Similarly to what happens in the quaternary borocarbides, we find that superconductivity coexists with a variety of magnetic arrangements of the local moments, ranging from commensurate to incommensurate spin-density waves, up to a critical value J_c(U); the conduction electrons show strong antiferromagnetic fluctuations in this region. Superconductivity is then suppressed by the appearance of a magnetic state with broken rotational symmetry in both the local-moment and itinerant electrons subsystems, so that for sufficiently strong J_c, a spiral-ferromagnetic ground state evolves to a ferromagnetic one.

1:27PM B33.00012 Alpha particle spectrometry using superconducting microcalorimeters

ROBERT HORANSKY, JOEL ULLOM, JAMES BEALL, GENE HILTON, GREGORY STEIHL, KENT IRWIN, NIST, ALEXANDER PLIONIS, STEPHEN LAMONT, CLIFFORD RUDY, MICHAEL RABIN, LANL — Alpha spectrometry is the preferred technique for analyzing trace samples of radioactive material because the alpha particle flux can be significantly higher than the gamma-ray flux from nuclear materials of interest. Traditionally, alpha spectrometry is performed with Si detectors whose resolution is at best 8 keV FWHM. Here, we describe the design and operation of a microcalorimeter alpha detector with an energy resolution of 1.06 keV FWHM at 5 MeV. We demonstrate the ability of the microcalorimeter to clearly resolve the alpha particles from Pu-239 and Pu-240, whose energy of separation is less than 13 keV. We also show the first direct observation of the decay of Pu-239 to the ground state of Pb-205 which has traditionally been obscured by a much stronger alpha line 2 keV away. Finally, the 1.06 keV resolution observed for alpha particles is far worse than the 0.12 keV resolution predicted from thermal fluctuations and measurement of gamma-rays. The cause of the resolution degradation may be ion damage in the tin. Hence, alpha particle microcalorimeters may provide a novel tool for studying ion damage and lattice displacement energies in bulk materials.

1:39PM B33.00013 High Resolution Gamma-Ray Spectroscopy with Superconducting Microcalorimeters

D.A. BENNETT, NIST, J.N. ULLOM, W.B. DORIESE, J.A. BEALL, G.C. HILTON, R.D. HORANSKY, K.D. IRWIN, N. JETHAVA, E. SASSI, L.R. VALE, NIST, M.K. BACRANIA, A.S. HOOVER, N. HOTELING, P.J. KARPIUS, M.W. RABIN, C.R. RUDY, D.T. VO, Los Alamos National Laboratory — We are currently developing high resolution gamma-ray microcalorimeters (µCal) for improved analysis of nuclear materials. The µCal consist of a bulk superconducting absorber attached to a transition-edge sensor (TES) biased in its resistive transition and operated at temperatures near 0.1 K. Incoming particles and photons are converted to heat in the absorber and the resulting temperature change is measured by the highly sensitive TES thermometer. The unmatched energy resolution of these devices is useful for nuclear safeguards. A specific application is the determination of Pu isotopics in complex mixtures. Although much of our effort is focused on the construction and multiplexed readout of large arrays of detectors for increased collection area, we are also working on optimizing the performance of individual pixels. To this end, we have developed an analytic µCal model that includes the thermal properties of the attached absorber and the large inductance in the TES circuit bias. We show how this model can be used to maximize the number of sensors that can be multiplexed into a single readout channel and to minimize the response time of individual sensors.

1:51PM B33.00014 In situ measurement of the permittivity of helium using microwave NbN resonators

LOREN SWENSEN, GRIGORIJ GRABOVSKIJ, OLIVIER BUISSON, CHRISTIAN HOFFMANN, ALESSANDRO MONFARDINI, Institut Neel, CNRS - Grenoble, France and University Joseph Fourier. JEAN-CLAUDE VILLEGIER, CEA-INAC, CEA - Grenoble, France — Due to their high quality-factors and ease of fabrication, superconducting microwave resonators are increasingly being recognized as ideal sensors in ultra-sensitive, low-temperature measurements. In this talk, we will discuss the design and characterization of superconducting NbN quarter-wave resonators implemented as a high-speed and spatially-sensitive detector for the permittivity of a surrounding helium bath. Measurements of a device with a ~10^{-11} mm^3 spatial resolution, a ~6×10^{-11} μ/Hz^{1/2} sensitivity to changes in the permittivity of helium, and a bandwidth of 300 kHz will be presented in the temperature range from 1.8 to 8.8 K. Potential applications, including operation as a fast, localized helium thermometer and as a transducer in superfluid hydrodynamic experiments, will be discussed.
2:03PM B33.00015 Instabilities and nonlinearities in the elastic vortex solid\textsuperscript{1}. SATYAJIT BANERJEE, SHYAM MOHAN, JAIVARDHAN SINHA, Department of Physics, Indian Institute of Technology, Kanpur-208 016, U. P., India, S. RAMAKRISHNAN, A. K. GROVER, AJAY SOOD, Department of Physics, Indian Institute of Science, Bangalore 560012, India — In recent times the influence of microscopic disorder has been viewed to play a crucial role in determining the configuration of vortices inside superconductors. Our recent investigations into the dissipation properties of the driven vortices\textsuperscript{[1]}, have found the existence of possible symmetry changes deep within the well ordered elastic vortex solid\textsuperscript{[1]}. The result is significant, as it requires a deeper revision of understanding the properties of the so called ‘benign’ elastic vortex solid. We have also studied the nonlinear properties of the driven elastic vortex solid\textsuperscript{[2]} through a random pinning environment and have found interesting highly nonlinear fluctuation in the time domain. We believe our results indicate the presence of process deep within the elastic driven phase which is a precursor to the plastic transformation in the vortex matter. \textsuperscript{[1]} Shyam Mohan, Jaivardhan Sinha, S. S. Banerjee\textsuperscript{a}, and Yuri Myasoedov, Phys. Rev. Lett. 98,027003 (2007). \textsuperscript{[2]} Shyam Mohan, Jaivardhan Sinha, S. S. Banerjee\textsuperscript{a} A. K. Sood, S. Ramakrishna, A. K. Grover (submitted, 2008) *satyajit@iitk.ac.in

3SSB acknowledges funding support from CSIR and DST, India.

**Monday, March 16, 2009 11:15AM - 2:03PM — Session B34 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors II: Quantum Oscillations, Electronic Structure and Magnetism 404**

11:15AM B34.00001 Fermi surface of superconducting LaFePO determined from quantum oscillations\textsuperscript{1}. AMALIA COLDEA, J. FLETCHER, A. CARRINGTON, Bristol University, J. ANALYTIS, Stanford University, C. ANDREW, A. BANGURA, Bristol University, J.-H. CHU, A. ERICKSON, I. FISHER, Stanford University, N. HUSSEY, Bristol University, R. MCDONALD, NHMFL, Los Alamos National Laboratory — We report extensive measurements of quantum oscillations in the normal state of LaFePO, using low temperature torque magnetometry and transport in high static magnetic fields (45 T). LaFePO is a bulk Fe-based superconductor (Tc~ 6 K) which can be grown in high quality single crystalline form being isostructural to LaFeAsO but without being affected by magnetic or structural transitions at low temperatures. We find that the Fermi surface is that of a compensated metal in broad agreement with the band-structure calculations with frequencies varying between 2.8% to 9% of the basal plane angle of the Brillouin zone. The effective masses vary between 1.7-2.1 me and the electronic correlations in LaFePO are moderate corresponding to a mass enhancement of about ~2. The observed variation in the electronic scattering between different bands may be related to their different orbital character. The quasi-two dimensional Fermi surface consists of nearly-nested electron and hole pockets, suggesting proximity to a spin/charge density wave instability. The upper critical field anisotropy is a factor ~10 (at 0.325 K) which may linked to its increased two-dimensionality (PRL 101, 216402 (2008)).

\textsuperscript{1}Financial support from Royal Society, EPSRC, DOE and NSF.

11:27AM B34.00002 Quantum Oscillations in the parent pnictide BaFe2As2: Fermi surface reconstruction of the magnetic ground state\textsuperscript{1}. JAMES ANALYTIS, Stanford Linear Accelerator Center, JUIN-HAW CHU, IAN FIRSHER, Stanford University, ROSS MCDONALD, Los Alamos National Laboratory, IGOR MAZIN, Naval Research Lab, ROSS MCDONALD COLLABORA- TION — We have measured quantum oscillations in the magnetically ordered ground state of BaFe2As2, a parent compound of the superconducting ternary pnictides. Measurements were performed in 65T pulsed field at the Los Alamos National High Magnetic Field Laboratory, using an atomic force microscope torque cantilever. We also perform detailed band-structure calculations for the spin-density wave ground state and find agreement with our observations of small quasi-two dimensional pockets. These results place significant constraints on our understanding of the magnetism associated with the Fe-As layers and layers that coherently quasiparticles persist in the magnetic ground state, providing an important clue about the nature of superconductivity which emerges when this compound is doped.

\textsuperscript{1}Department of Energy

11:39AM B34.00003 Quantum oscillations in the parent magnetic phase of an iron arsenide high temperature superconductor\textsuperscript{1}. NEIL HARRISON, Los Alamos National Laboratory, SUCHITRA SEBASTIAN, J. GILLET, P. LAU, Cavendish Laboratory, Cambridge, DAVID SINGH, Oak Ridge National Laboratory, CHARLES MIELKE, Los Alamos National Laboratory, GILBERT LONZARICH, Cavendish Laboratory, Cambridge — We report quantum oscillation measurements in SrFeAsF at temperatures which is known to become superconducting under doping and pressure. The magnetic field and temperature dependences of the oscillations between 20 and 55 T suggest that the electronic excitations are those of a Fermi liquid. We show that the observed Fermi surface comprising small pockets is consistent with the formation of a spin-density wave. Our measurements thus demonstrate that high Tc superconductivity can occur on doping or pressurizing a conventional metallic spin-density wave state.

\textsuperscript{1}DOE, NSF, Florida State and UK EPSRC are al acknowledged

11:51AM B34.00004 Fermi surface changes in LaFeAsO\textsubscript{1-x}F\textsubscript{x} using supercells, rigid band shifts, and the virtual crystal approximation\textsuperscript{1}. PAUL LARSON, University of Nebraska, SASHI SATPATHY, University of Missouri — There is currently great interest in the properties of the superconducting material LaFeAsO. While numerous calculations have been performed for this material, questions arise about which theoretical description in the Fermi surface with doping. We have performed ab initio density functional studies of F-doping in the non-magnetic state using supercell calculations and compared these results to those obtained using rigid band shifts and the virtual crystal approximation (VCA). The Fermi surface consists mainly of Fe d and As p states with La and O states lying far from the Fermi level. Significant differences are found by comparing the supercell results with those of the rigid band shifts, but remarkable agreement is found for the Fermi surface using VCA calculations where the reconstruction of the magnetic ground state.

\textsuperscript{1}This work is supported by DE-FG02-00ER45818.

12:03PM B34.00005 Momentum density, Fermi surface and directional Compton profile in the iron-based superconductor LaOFe\textsubscript{As} , Y. J. WANG, HSIN LIN, B. BARBIELLINI , Northeastern U., P. E. MUNARENS, Northeastern U. and U. Tech., Delft, The Netherlands, S. KAPRZYK, Northeastern U. and Academy of Mining and Metallurgy AGH, Poland, W. AL-SAWAI, R.S. MARKIEWICZ, A. BANSIL, Northeastern U. — We have carried out first principles all-electron calculations of the (001) projected 2D electron momentum density (2D-EMD) and directional Compton profiles (CPs) along the [100], [001], and [110] directions in iron-based superconductor LaO\textsubscript{1-x}F\textsubscript{x}Fe\textsubscript{3} for various doping concentrations x within the framework of the local density approximation (LDA). We have identified Fermi surface features both in the 2D-EMD and in the CPs. Bonding effects related to the character of wave functions near the Fermi level are revealed by the autocorrelation function B(r) defined as the Fourier transform of the momentum density. Work supported in part by the US Department of Energy.
12:15PM B34.00006 First Principles studies of 122 Ferropnictide Surface1, ALEXANDER KEMPER, P.J. HIRSCHFELD, H-P. CHENG, University of Florida — We present DFT-GGA calculations for the Ba and Sr-122 ferropnictide materials on the effect of surfaces on the electronic structure. It has been established that there is a strong modulation of the electronic structure by the Fe-As distance, which decreases near a free surface due to surface reconstruction. Indeed, we see significant changes of both Fermi velocities and Fermi surfaces due to these effects for both the paramagnetic and collinear spin density wave states. These changes of the electronic structure, which we exhibit here, will be crucial for the interpretation of surface probes like ARPES and STM.

1DOE DE-FG02-02ER45995 and DOE-BES DE-FG02-05ER46236.

12:27PM B34.00007 Structural, spin, and orbital phase transitions in LaOFeAs: I. Total energy calculations. WEI KU, CHI-CHENG LEE, WEI-GUO YIN, Brookhaven National Laboratory — Recent experimental studies on iron pnictides showed the existence of local Fe magnetic moments even in the superconducting phase, indicating strong fluctuations in a short time scale. We report a investigation of the local electron-lattice and electron-spin couplings via total energy calculations within first-principles density functional theory. Strong coupling in both channels were found to be closely tied to a ferro-orbital order, which drives the structure transition and the stripy magnetic (SDW) transition at high temperature in the undoped system. We suggest that this orbital degree of freedom leads to stronger coupling upon doping and thus possible enhancement of superconductivity.

12:39PM B34.00008 Structural, spin, and orbital phase transitions in LaOFeAs: II. Wannier function analysis , WEI-GUO YIN, CHI-CHENG LEE, WEI KU, Brookhaven National Laboratory — A realistic low-energy effective interacting Hamiltonian of doped LaOFeAs is derived quantitatively from a novel first-principles Wannier function analysis. Strong local orbital, spin, and lattice coupling to the doped charge is found associated with the orbital degree of freedom, which suggests a possible explanation of the high transition temperature. The fluctuations in the orbital sector fundamentally distinguish the iron pnictides from the copper oxide superconductors, and ensure the essential role of phonons in the mechanism of superconductivity in this new class of materials, in addition to electronic origin.

12:51PM B34.00009 Emergence of complex magnetism in three dimensional, yet quasi-layered, iron pnictides: CaFe$_2$As$_2$1, ARTHUR J. FREEMAN, GIANCARLO TRIMARCHI, MERCOURI KANATZIDIS, Northwestern U.. ILYA TODOROV, DUCK-YOUNG CHUNG, Materials Science Division, ANL, Argonne IL 60439 — The class of iron pnictides has been the focus of much attention for the discovery of superconductivity in the layered compounds LaOFeAs, CaFe$_2$As$_2$, and related ones; the phase diagrams of these pnictides remain still largely unexplored. Here, we report on the electronic and magnetic structure of the recently synthesized CaFe$_2$As$_2$ compound. This material, as opposed to the layered CaFe$_2$As$_2$, shows FeAs slabs parallel to the $b$-direction and approximately perpendicular to each other, defining tunnels filled by the Ca atoms. No sign of superconductivity was found in this compound. Instead, the system shows a complex ferromagnetic state at low temperature. DFT calculations performed on the refined crystal structure using the highly precise FLAPW method show a pronounced stabilization for the ferromagnetic state which is characterized by four distinct Fe sites with magnetic moments of between 1 $\mu_B$ and 2 $\mu_B$. The influence of the local topology of the crystal structure on the the electronic and magnetic state is analyzed.

1Supported by DOE (grant No. DE-FG02-88ER45372).

1Wimmer, Krakauer, Weinhart, and Freeman, PRB, 24, 864 (1981)

1:03PM B34.00010 ‘Unscreening’ Effect on Fe-Pnictide Superconductor, MASAO OGATA, Department of Physics, University of Tokyo and JST, TRIP, YUKI FUSEYA, TOSHIIKAZE KARIYADO, Department of Physics, University of Tokyo — We study a microscopic mechanism of Fe-pnictide superconductor, considering the screening effects of Coulomb interaction in addition to the conventional spin-fluctuation mechanism. It is shown that, by electron doping, the transition temperature of superconductivity increases due to the ‘unscreening’ effect even though the density of states decreases, while that of spin-density wave rapidly decreases due to breaking of nesting conditions. Our results give a clear interpretation to the mystery of interrelation between $T_c$ and the density of states observed in the Fe-pnictide superconductors.

1:15PM B34.00011 Quasiparticle scattering interference in superconducting Oxypnictides . YANYANG ZHANG, KANGJUN SEO, XIATING ZHOU, Purdue University, B. ANDREI BERNEVIG, Princeton University, JIANGPING HU, Purdue University — Based on a two-band model of the superconducting iron oxypnictides, we study the effects of single-impurity scattering on the local density of states by exact T-matrix calculations. We compare the quasi-particle interference patterns in different pairing states, as well as different kinds of impurities. The results of this calculation can be used to test and distinguish different sorts of pairing symmetries and impurities in the experiments.

1:27PM B34.00012 Quasi-particle properties in iron-based superconductors1, XIANG HU, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — The pairing symmetry is one of the major issues in the study of iron-based superconductors. We adopted a minimum two band model, to introduce the two-band Bogoliubov de Gennes equations. By solving those equations numerically, we checked the possibilities of different pairing symmetry, and made some predictions which can be tested by future experiments in spectrum tunnelling microscopy.

1Supported by a grant from the Robert A. Welch Foundation, No. E-1146 and TcSUS, and under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DEAC52-06NA25396.

1:39PM B34.00013 Nature of the SDW state in FeAs-based Compounds , XI DAI, ZHONG FANG, GUANGTAO WANG, GANG XU, Institute of Physics, CAS, Beijing, China — We show that the significant underestimation (about 10%) of Fe-As bond length in FeAs-based compounds by LDA is due to the strong correlation effect. By properly taking into account the on-site correlation, we are able to reproduce experimental values (to about 1%) using self-consistent LDA+Gutzwiller method. Also we will show that the strong on-site orbital fluctuation will dramatically reduce the anti-ferromagnetic long range order in the parent compound. All these results are in good agreement with experiments.

1:51PM B34.00014 High-temperature Superconductivity: Status . JOHN D. DOW, Physics Department, Arizona State University, Tempe, AZ. DALE R. HARSHMAN, Physikon Research Corporation, P.O. Box 1014, Lynden, WA 98264. ANTHONY R. FIORY, Physics, New Jersey Institute of Technology, Newark, NJ 07102 — A theory of high-temperature superconductivity is presented which (i) explains the cuprates, with cuprate-planes; (ii) describes the superconducting ruthenates without cuprate-planes, such as Ba$_2$YRuO$_6$; (iii) treats the rutheno-cuprates, such as GdSr$_2$Cu$_2$RuO$_6$, whose cuprate-planes do not superconduct; (iv) treats the molecule $\kappa$-[BEDT-TTF]$_2$Cu$_2$[NC$_2$]$_3$ which superconducts via S, and (v) explains the pnictides. In YBa$_2$Cu$_3$O$_y$, the theory is consistent with the observation that no Cu-containing plane superconducts and the observed superconductivity is $\kappa$-wave, not $\delta$-wave, once fluxon-de-pinning has been properly accounted for. The superconducting layers are BaO layers, in $\kappa$-type, and are adjacent to the $\lambda$-type cuprate-planes. The theory is consistent with many data which were previously beyond explanation.
11:15AM B35.00001 Valley density-wave (VDW) and Superconductivity in Iron-Pnictides
Vladimir Cvetkovic, Zlatko Tesanovic, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD — One of the experimentally observed features of iron-pnictide superconductors is the structural transition and SDW ordering occurring at almost the same temperature. Starting from a tight-binding model [1], we construct an effective theory for iron-pnictides with the distinctive two hole and two electron Fermi surfaces. This theory is then mapped onto a negative-U Hubbard model with additional orbital and spin flavors [2]. We demonstrate that the superconducting instability of the attractive Hubbard model — valley density-wave (VDW) — corresponds to the observed structural and SDW orders. The deviations from perfect nesting between the hole and electron Fermi surfaces are mapped onto the Zeeman field which causes partial Fermi surface to remain ungapped. The origin of pnictide superconductivity in this model, and its ties to the VDW are discussed. [1] V. Cvetkovic and Z. Tesanovic, http://arxiv.org/abs/0804.4678. [2] V. Cvetkovic and Z. Tesanovic, http://arxiv.org/abs/0808.3742.

11:27AM B35.00002 Spin-Density Wave in Iron Pnictides
Jian Kang, Valentin Stanev, Zlatko Tesanovic, Johns Hopkins University — Multi-band Hubbard-like model with appreciable nesting is applied to the study of spin-density wave (SDW) in iron pnictides: $\text{Fe}_x\text{Co}_y\text{As}_2$. It is assumed that the SDW particle-hole pairing mechanism arises from the short range interaction between hole bands near $\Gamma$ point and electron bands near M. Within the Hubbard-Stratonovich transformation, an auxiliary field is introduced to obtain the effective action. The mean-field solution is obtained by the stationary phase analysis of this action, and results in an itinerant, antiferromagnetically ordered ground state, with the staggered magnetic moment modulation at wavevector $\mathbf{M}$. We study fluctuations of the spin order around $\mathbf{M}$, both in its direction and amplitude. We present detailed results for the propagation velocity of this mode (spin-wave velocity) as a function of the various parameters of our model and compare them to the available experimental observations of the spin-wave spectrum.

11:39AM B35.00003 Iron-based superconductors: What can we learn from DFT?
Lilja Boeri, Oleg Dolgov, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany, Alexander Golubov, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands, Ole Krogh Andersen, Max-Planck-Institute for Solid State Physics, Stuttgart, Germany — The discovery of superconductivity in iron pnictides has initiated an intense theoretical activity. So far, however, not only the pairing mechanism, but even the basic electronic structure of these materials is not well understood. We use Density Functional Theory to understand the electronic and vibrational properties of LaOFeAs, which can be considered a prototype for iron pnictides. First, we calculate the phonon dispersions and electron-phonon coupling using linear response and show that standard Migdal-Eliashberg theory cannot explain the experimental Tc. Then we derive ab-initio an accurate tight-binding Hamiltonian, using downfolding + N-ization (NMTO), which allows us to elucidate the origin of the complicated band structure of iron pnictides. As a first application of our model, we study magnetism.

11:51AM B35.00004 Correlations in Ferropnictides
Klaus Koepernik, IFW Dresden, Germany, Helmut Eschrig, IFW Dresden, Germany — The strength of correlations in the ferropnictide superconductors is still under debate. While arguments for an electron-electron interaction $U$ of 5eV have been made, some experimental results support a $U$ of merely 1eV. Density functional theory in the local spin density approximation (LSDA) seems to describe several aspects of the electronic structure quite reasonably, which would also support a smaller $U$. However, the unusually large error of the calculated lattice structure remains a puzzle. We discuss the influence of correlations on the electronic structure and the properties of the ferropnictides in the framework of LSDA+U calculations.

12:03PM B35.00005 Superconductivity in SrFe$_2$-Co$_x$As$_2$: Internal Doping of the Iron Arsenide Layers
Helge Rosner, Andreas Leithe-Jasper, Walter Schnelle, Christoph Geibel, MPI CPfS Dresden — In the strontium iron-cobalt arsenides SrFe$_{2-x}$Co$_x$As$_2$ ($0.2 \leq x \leq 0.4$) superconductivity with Tc up to 20 K is observed in magnetic susceptibility, electrical resistivity, and specific heat data. This first observation of bulk superconductivity induced by electron doping in this family of compounds — despite strong disorder in the Fe-As layer — is strongly enhanced compared to an ordinary Fermi liquid as it contains precisely the same interaction that gives rise to spin-density-wave ordering. We compare theoretical slope with the data.

12:15PM B35.00006 Linear temperature dependence of the spin susceptibility in Fe-pnictides
Dmitri V. Efremov, Andrei V. Chubukov, Ilya M. Eremin, Maxim M. Korsunov, Dmitri L. Maslov — We argue that linear T dependence of the spin susceptibility $\chi$ > 0 observed in Fe-pnictides can be explained within the itinerant Fermi liquid model of hole and electron bands. The spin susceptibility is linear in T in a generic Fermi liquid in 2D. We show that for pnictides, the prefactor of the T term comes chiefly from intra-band scattering and is strongly enhanced compared to an ordinary Fermi liquid as it contains precisely the same interaction that gives rise to spin-density-wave ordering. We compare theoretical slope with the data.

12:27PM B35.00007 Theory of novel and superconducting properties of Fe-based superconductors
Andrey Chubukov, University of Wisconsin — I will discuss antiferromagnetism and superconductivity in novel Fe-based superconductors within the itinerant model of small electron and hole pockets near (0,0) and (π,π). I will argue that the effective interactions in both channels logarithmically flow towards the same values at low energies, i.e., antiferromagnetism and superconductivity must be treated on equal footing. The magnetic instability comes first for equal sizes of the two pockets, but looses to superconductivity upon doping. The superconducting gap has no nodes, but changes sign between the two Fermi surfaces (extended s-wave symmetry). I will argue that the T dependence of the spin susceptibility, NMR relaxation rate, and the penetration depth for such state are exponential only at very low T, and can be well fitted by power-laws over a wide T range below $T_c$. I will also discuss the type of a transition between spin-density-wave and superconducting states at $T = 0$ and at finite $T$, and the linear T dependence of the spin susceptibility in the normal state. Based on the works done with I. Eremin, D. Efremov, M. Korsunov, D. Maslov, M. Vavilov, and A. Vorontsov.
while electrons in the lower level are more localized. The resulting magnetic moment is highly anisotropic with an in-plane value of the filling of the Fe d-levels. The two highest occupied levels have one electron each but as a result of differing p-d hybridizations, the upper level is more itinerant.

Department of Physics, University of Illinois at Urbana-Champaign, ANTONIO CASTRO-NETO, Department of Physics, Boston University — We show that different chiralities (both metallic and semiconducting) remain metallic for beyond n=3, with conductance close to 4e

the appearance of a number of new bands in the electronic structure, especially near the Fermi level. These new bands serve to modify the density of states near optimization shows that Pt prefers to form clusters rather than spread out and "wet" the SWNTs. Atom-by-atom increase in the cluster size is associated with density functional theory to investigate the structure and electronic properties of Pt nanocluster decoration of single-wall carbon nanotubes (SWNTs). Energy

we set interaction parameters appropriately.

Nanotubes

2

yet, much as in polymer science and engg, such applications require appropriate fluid based dispersions which can undergo industrial processing that translate properties of elemental molecules (SWNTs) into macroscopic materials. We report a detailed study on the flow behavior of aqueous SWNT dispersions.

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respective transparency of 70% and 90%). The results presented here, both in terms of scientific understanding of how to control fluid and process, and in terms of a scalable technique, paves the way to the deployment of transparent conductive SWNT films in large scale commercial applications.

1

and optical microscopy. A SWNT-SDBS-TritonX100 dispersion was found to have the appropriate viscoelastic and shear thinning behavior for rod roll-to-roll (rod based) thin film coating process. Purified, pristine SWNTs were dispersed in water at high concentrations using surfactants and analyzed using rheology and optical microscopy. A SWNT-SDBS-TritonX100 dispersion was found to have the appropriate viscoelastic and shear thinning behavior for rod coating. Rod coating, washing and sulfuric acid treatment resulted in highly uniform thin films of pure SWNT (sheet resistance of 100 and 300 \Omega/sq for respective transparency of 70% and 90%). The results presented here, both in terms of scientific understanding of how to control fluid and process, and in terms of a scalable technique, paves the way to the deployment of transparent conductive SWNT films in large scale commercial applications.

1:03PM B35.00008 Nodal Spin Density Wave and band topology of the FeAs based materials . HUI ZHAI, LBL, UC Berkeley, YING RAN, FA WANG, ASHVIN VISHWANATH, DUNG-HAI LEE, UC Berkeley — The recently discovered FeAs-based materials exhibit a \((\pi,0)\) Spin Density Wave (SDW) in the undoped state, which gives way to superconductivity upon doping. Here we show that due to an interesting topological feature of the band structure, the SDW state cannot acquire a full gap. This is demonstrated within the SDW mean-field theory of both a simplified two band model and a more realistic 5-band model. The positions of the nodes are different in the two models and can be used to detect the validity of each model.

1:15PM B35.00009 Normal State Spin Dynamics of Five-band Model for Iron-pnictides . TOSHIKAZE KARIYADO, MASAO OGATA, Department of Physics, University of Tokyo and JST, TRIP — Normal state (assuming absence of SC or AF order) spin dynamics of iron-pnictide superconductors is discussed by calculating spin structure factor \(S(q,\omega)\) in an itinerant five-band model within RPA approximation. Due to the characteristic Fermi surface structure of iron-pnictide, column like response is found at \((\pi,0)\) in extended Brillouin zone. This is consistent with recent neutron experiments. Furthermore, we show that the temperature dependence of inelastic neutron scattering intensity is reproduced if we set interaction parameters appropriately.

1:27PM B35.00010 Symplectic fermion approach to the striped magnetism in the iron arsenides , XUN XUE, East China Normal University, JIANHUI DAI, Zhejiang Modern Physics Center — Based on the fact that the near transition temperature of striped SDW and structure distortion in iron pnictides, we propose a symplectic fermion approach to account for this kind of antiferromagnetic properties. The model is expecting for better understanding of the experimental results.

1:39PM B35.00011 Parquet formalism applied to pnictide superconductors , JUN LIU, KARLIS MIKELSONS, SHUXIANG YANG, HERBERT FOTSO, MARK JARRELL, Louisiana State University — DMFT combined with Parquet approximation is used to study the single particle property of pnictide superconductors (such as FeSe, SrFe2As2,...) in an attempt to understand the enhancement of superconductivity under pressure. By tracking the evolution of one-particle spectral function, pressure dependence of this type of compound is studied in depth. In the study, inhomogeneous frequency grid is used to high frequency summation.

1:51PM B35.00012 Jahn-Teller Effect, Structural Phase Transition and Resistivity Anomaly in Iron Pnictides , WEICHENG LV, JIANSHENG WU, PHILIP PHILLIPS, University of Illinois — We attribute the structural phase transition (SPT) in the parent compounds of iron pnictides to a Jahn-Teller distortion. Due to the anisotropy of the \(d_{xz,\pi}\) and \(d_{yz,\mu}\) orbitals in the \(xy\) plane, some orbital ordering will make the orthorhombic structure more energetically favorable, thus inducing the SPT. In an orbital ordered system, the sites with orbitals that do not order act as scattering impurities, causing a resistivity anomaly upon the onset of the SPT. Below the SPT, we find that the resistivity displays a \(lnT\) divergence. All of these are in agreement with the experiments.

2:03PM B35.00013 Theory of the Magnetic Moment in Iron Pnictides1, JIANSHENG WU, PHILIP PHILLIPS, Department of Physics, University of Illinois at Urbana-Champaign, ANTONIO CASTRO-NETO, Department of Physics, Boston University — We show that the combined effects of spin-orbit, monoclinic distortion, and p-d hybridization in tetrahedrally coordinated Fe in \(LaFeAsO\) invalidates the naive Hund’s rule filling of the Fe d-levels. The two highest occupied levels have one electron each but as a result of differing p-d hybridizations, the upper level is more itinerant while electrons in the lower level are more localized. The resulting magnetic moment is highly anisotropic with an in-plane value of 0.25 – 0.35\(\mu_B\) per Fe and a z-projection of 0.06\(\mu_B\), both of which are in agreement with experiment.

1 P.P. was supported in part by the NSF DMR-0605769.


11:15AM B36.00001 Density Functional Theory Design of All-metallic Single-wall Carbon Nanotubes2, LI CHEN, SWASTIK KAR, SAROJ NAYAK, Rensselaer Polytechnic Institute, PULICKEL AJAYAN, Rice University — We have used density functional theory to investigate the structure and electronic properties of Pt nanocluster decoration of single-wall carbon nanotubes (SWNTs). Energy optimization shows that Pt prefers to form clusters rather than spread out and "wet" the SWNTs. Atom-by-atom increase in the cluster size is associated with the appearance of a number of new bands in the electronic structure, especially near the Fermi level. These new bands serve to modify the density of states near the Fermi level. While metallic SWNTs remain metallic, semiconducting SWNTs lose their band-gap rapidly with the inclusion of more than 3 atoms per cluster, and continue to remain metallic for all tested cluster sizes \((n=0-13\) and 19). Room temperature \((T=300K)\) calculations of conductance show that SWNTs of different chiralities (both metallic and semiconducting) remain metallic for beyond \(n=3\), with conductance close to 4e\(^2\)/h. In some cases, the conductance is found to exceed this value. This gives an easy for designing “all-metallic” SWNT bundles.

2 Acknowledgement: Interconnect Focus Center at RPI (part of an FCRP of SRC)

11:27AM B36.00002 Designing of Single Walled Carbon Nanotubes dispersions for industrial scale processing and roll-to-roll coating applications . BUDDHADIPTA DAN, MATTEO PASQUALI, Rice University — Carbon nanotubes (CNTs) combine nanoscale size with high aspect ratio and unique properties, making them ideal candidate materials for high-impact applications. Yet, much as in polymer science and engg, such applications require appropriate fluid based dispersions which can undergo industrial processing that translate the properties of elemental molecules (SWNTs) into macroscopic materials. We report a detailed study on the flow behavior of aqueous SWNT dispersions involving surfactants, its dependence on SWNT & surfactant concentration, and type of surfactant. We also design a SWNT dispersion for use in industrial roll-to-roll (rod based) thin film coating process. Purified, pristine SWNTs were dispersed in water at high concentrations using surfactants and analyzed using rheology and optical microscopy. A SWNT-SDBS-TritonX100 dispersion was found to have the appropriate viscoelastic and shear thinning behavior for rod coating. Rod coating, washing and sulfuric acid treatment resulted in highly uniform thin films of pure SWNT (sheet resistance of 100 and 300 \Omega/sq for respective transparency of 70% and 90%). The results presented here, both in terms of scientific understanding of how to control fluid and process, and in terms of a scalable technique, paves the way to the deployment of transparent conductive SWNT films in large scale commercial applications.
Characteristics. The quality of suspended CNTs is characterized by electrical transport as well as 1/f noise measurements. Standard resist-processed CNTs demonstrated by controlling the number of suspended CNTs per device, and by re-using the same electrode set multiple times to produce the desired device. A printing process is used to transfer CVD-grown CNTs onto specially configured electrode (Au) sets fabricated on SiO₂ methods have been developed to fabricate suspended carbon nanotube (CNT) field effect transistors using as-grown CNTs without subsequent chemical processing.

Devices

∼ 2 wafers using our facile transfer printing method. 2) Wafer-scale device fabrication was performed on 4 inch Si/SiO₂ arrays for high performance submicron channel transistors and integrated nanotube circuits, including the following essential components. 1) The massively aligned carbon nanotube (swCNT) networks were extensively studied for various practical applications such as transistors, sensors, etc. However, those devices have been suffering various limitations such as poor on-off ratio due to metallic swCNTs in the networks, decreased mobility and conductance for devices with reduced linewidth due to the percolation problem, etc. Herein, we present a simple but efficient strategy to significantly improve the performance of swCNT network devices. 1) Massively aligned nanotubes can be improved by increasing the density and alignment of tubes and avoiding the problems associated with random networks. We are optimizing this approach by preparing devices composed of parallel arrays of CNTs fabricated on quartz and plastic substrates. CNT growth catalysts, ferric nitrate, ferritin and iron, are a pair of control of the degree and alignment of the grown tubes. Though ferric nitrate produced a denser network, ferritin allows a high degree of alignment, and iron will also be used. Plastic devices with a 5 µm channel length and a 22.5 mm width were prepared with approximately 1 channel crossing tube per 4 µm of width. The density is improved by repeatedly printing more CNT’s to the same area. The metallic tubes were removed by selective electrical breakout, marginally increasing the on/off current ratio while decreasing the On current from 800µA to 450µA (at Vgs=−20V, Vds=−10V). Results from optimized devices prepared with patterned iron as the growth catalyst will also be presented.

11:15AM B36.00006 Transfer Printed Parallel Carbon Nanotube Devices¹, ANDREW TUNELL, VINO SANGWAN, VINCENT BALLAROTTO, DANIEL HINES, MICHAEL FUHRER, ELLEN WILLIAMS, University of Maryland — Carbon nanotube (CNT) device properties can be improved by increasing the density and alignment of tubes and avoiding the problems associated with random networks. We are optimizing this approach by preparing devices composed of parallel arrays of CNTs fabricated on quartz and plastic substrates. CNT growth catalysts, ferric nitrate, ferritin and iron, are a pair of control of the degree and alignment of the grown tubes. Though ferric nitrate produced a denser network, ferritin allows a high degree of alignment, and iron will also be used. Plastic devices with a 5 µm channel length and a 22.5 mm width were prepared with approximately 1 channel crossing tube per 4 µm of width. The density is improved by repeatedly printing more CNT’s to the same area. The metallic tubes were removed by selective electrical breakout, marginally increasing the on/off current ratio while decreasing the On current from 800µA to 450µA (at Vgs=−20V, Vds=−10V). Results from optimized devices prepared with patterned iron as the growth catalyst will also be presented.

1) Work supported by the NRL and TND programs.

11:27PM B36.00007 ABSTRACT WITHDRAWN

12:03PM B36.00005 Fabricating Substrates to Combine Electron Microscopy and Diffraction with Electrical Characterization of Single and Double-Walled Carbon Nanotubes, SCOTT PAULSON, LOK-KIN TSUI, JOSEPH HARCASSEL, James Madison University — Carbon nanotubes based electronics make model systems for pursuing electronic devices at the nanometer scale. They are chemically robust, and have well defined easily predictable electronic structure. However, device integration requires not just an understanding of the nanotube properties, but also the properties of interfaces between neighboring elements. Ideally the structure-property relationship of the interface between two nanotubes would consist of complete electrical characterization coupled with atomic scale structural information. The former is achieved by lithographic patterning of a nanotube into a circuit, the latter through high resolution TEM imaging and diffraction. Unfortunately, typical TEM preparation of nanotubes is not compatible with lithographic processing and vice-versa. In this talk we will present a fabrication process that integrates carbon nanotubes into devices on a TEM compatible substrate. Sample devices will be shown, and preliminary data will be presented.

12:15PM B36.00006 Transfer Printed Parallel Carbon Nanotube Devices¹, ANDREW TUNELL, VINOD SANGWAN, VINCENT BALLAROTTO, DANIEL HINES, MICHAEL FUHRER, ELLEN WILLIAMS, University of Maryland — Carbon nanotube (CNT) device properties can be improved by increasing the density and alignment of tubes and avoiding the problems associated with random networks. We are optimizing this approach by preparing devices composed of parallel arrays of CNTs fabricated on quartz and plastic substrates. CNT growth catalysts, ferric nitrate, ferritin and iron, are a pair of control of the degree and alignment of the grown tubes. Though ferric nitrate produced a denser network, ferritin allows a high degree of alignment, and iron will also be used. Plastic devices with a 5 µm channel length and a 22.5 mm width were prepared with approximately 1 channel crossing tube per 4 µm of width. The density is improved by repeatedly printing more CNT’s to the same area. The metallic tubes were removed by selective electrical breakout, marginally increasing the on/off current ratio while decreasing the On current from 800µA to 450µA (at Vgs=−20V, Vds=−10V). Results from optimized devices prepared with patterned iron as the growth catalyst will also be presented.

1) Work supported by the Lab for Physical Sciences, College Park, MD

12:27PM B36.00007 ABSTRACT WITHDRAWN

12:39PM B36.00008 Textured Network Devices: Overcoming Fundamental Limitations of Nanotube/Nanowire Network-based devices¹, MINBAEK LEE, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul Natl University, Seoul, Korea, MEG NOAH, YOUNG-KYUN KWON, Department of Physics and Applied Physics, University of Massachusetts, Lowell MA, USA, JUNE PARK, MAENG-JE SEONG, Department of Physics, Chung-Ang University, Seoul, Korea — Thin film devices based on single-walled carbon nanotube (swCNT) networks were extensively studied for various practical applications such as transistors, sensors, etc. However, those devices have been suffering various limitations such as poor on-off ratio due to metallic swCNTs in the networks, decreased mobility and conductance for devices with reduced linewidth due to the percolation problem, etc. Herein, we present a simple but efficient strategy to significantly improve the performance of swCNT network devices by controlling the network structures. In this strategy, surface molecular patterns were utilized to prepare swCNT network-based devices with desired connectivity. We will discuss systematic study about the effect of swCNT network connectivity, as well as enhancements of on-off ratio, mobility and conductance of textured network-based transistors.

¹The work was supported by the NRL and TND programs.

12:51PM B36.00009 CMOS-analogous wafer-scale nanotube-on-insulator approach for submicron devices and integrated circuits using aligned nanotubes, KOUCHMIN RYU, ALEXANDER BADMAEV, CHUAN WANG, CHONGWU ZHOU, University of Southern California — Massively aligned carbon nanotubes hold great potential but also face significant integration / assembly challenges for future beyond-silicon nanoelectronics. We report our recent advance on full wafer-scale processing of massively aligned carbon nanotube arrays for high performance submicron channel transistors and integrated nanotube circuits, including the following essential components. 1) The massively aligned nanotubes were successfully grown on 4 inch quartz and sapphire wafers via a unique temperature control, and then transferred onto Si/SiO₂ wafers using our facile transfer printing method. 2) Wafer-scale device fabrication was performed on 4 inch Si/SiO₂ wafer to yield submicron channel transistors and circuits with high on-current density ~ 20 µA/µm and good on/off ratio. 3) Chemical doping methods were successfully demonstrated to get CMOS inverters with a gain ~5. 4) Defect-tolerant circuit design for NAND and NOR was proposed and demonstrated to guarantee the correct operation of logic circuits, regardless of the presence of mis-aligned or mis-positioned nanotubes.

1:03PM B36.00010 A Novel Fabrication Method for Pristine Suspended Carbon Nanotube Devices², VINO SANGWAN, VINCENT BALLAROTTO, MICHAEL FUHRER, ELLEN WILLIAMS, University of Maryland — A simple and scalable method has been developed to fabricate suspended carbon nanotube (CNT) field effect transistors using as-grown CNTs without subsequent chemical processing. A printing process is used to transfer CVD-grown CNTs onto specially configured electrode (Au) sets fabricated on SiO₂. The versatility of the technique is demonstrated by controlling the number of suspended CNTs per device, and by re-using the same electrode set multiple times to produce the desired device characteristics. The quality of suspended CNTs is characterized by electrical transport as well as 1/f noise measurements. Standard resist-processed CNTs on SiO₂ substrates show p-type behavior and strong hysteresis associated with doping by the SiO₂ surface and charge trapping in the SiO₂., respectively. In contrast, suspended CNTs show ambipolar behavior with negligible hysteresis. Low frequency noise measurements on suspended CNT show 1/f behavior with Hooge’s constant 2.6 x 10⁻³, around 20 times less than that of CNTs lying on SiO₂, consistent with reduced effect of the SiO₂ charge traps, responsible for the bulk of the noise in CNTs on SiO₂.

²V. K. Sangwan et al, APL 93, 113112 (2008)
We present the observation of unidirectional electric current through as-grown single-walled carbon nanotubes (SWNTs) grown by catalytic chemical vapor deposition (CCVD) process. Long strands of as-grown SWNTs were utilized to fabricate multiple arrays of switching devices with the channel length of 3, 5, 7 and 10 μm on a 15 mm x 15 mm SiO₂ on Si substrate. Of the fabricated devices, ~ 34% exhibited electrical activity. Of the active devices, about 70% exhibited diode-like unidirectional current, not observed previously in CCVD grown SWNTs. High resolution atomic force microscopic (AFM) analysis of the device structure and surface topology of SWNTs suggests the observed unidirectional current to result from surface irregularities and change in the chirality along the tube axis.

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1:27PM B36.00012 Gate Controlled Negative Differential Resistance and Photoconductivity Enhancement in Carbon Nanotube Intra-connects. SEON WOO LEE, Electronic Imaging Center at NJIT and the Electrical and Computer Engineering Department, New Jersey Institute of Technology (NJIT), Newark, NJ 07102, SLAVA ROTKIN, Physics Department and CAMN, Lehigh University, Bethlehem, PA 18015, ANDREI SIRENKO, Physics Department, New Jersey Institute of Technology (NJIT), Newark, NJ 07102, HAIM GREBEL, Electronic Imaging Center at NJIT and the Electrical and Computer Engineering Department, New Jersey Institute of Technology (NJIT), Newark, NJ 07102. — Field effect transistors were fabricated using carbon nanotube (CNT). Gate-controlled, N-shaped negative differential resist (NDR) has been demonstrated. In addition, a large photoconductance effect was associated with the NDR. The intra-connects – bridges spanning across planar electrodes and contain individual tube or in a small bundle – were grown using chemical vapor deposition (CVD) precisely between very sharp metal tips on the pre-fabricated electrodes. NDR was observed for intra-connects exhibiting either, ohmic or, non-ohmic contacts. Yet, the enhanced photoconductivity was more pronounced for intra-connects exhibiting ohmic contact at zero gate bias.

1:39PM B36.00013 Magnetic Carbon Nanotubes: Materials Development and Property Characterization. DEREJE SEIFU, Department of Physics, Morgan State University, Baltimore, MD 21251, USA, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRD-ARL-WM, Aberdeen Proving Ground, MD 21005-5069, USA. — A versatile chemical method was used to fill multi-wall carbon nanotubes (MWNTs) with ferromagnetic nanoparticles [1]. For the first time, pulsed laser deposition and magnetron DC sputtering were used to fill vertically aligned MWNTs. The later approaches gave high-yield nanoparticle filling of MWNTs. Samples were characterized by Electron Microscopy, Energy Dispersive Spectroscopy, Mössbauer Spectroscopy, and magnetization measurements. Mössbauer measurements on chemically impregnated MWNTs clearly show the presence of atomic Fe as well as mixed phases of Fe nano-particles inside the tubes. Magnetization measurements on PLD-filled vertically aligned MWNTs indicate reasonable coercivity. However, the magnetic anisotropy appears to be randomly oriented, suggesting polycrystalline sample. Acknowledgement: The research at Morgan State University was partially supported by the US ARL-WMRD (W1813LT-5006-7056).

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1:51PM B36.00014 Electrical and Thermal Properties of Oriented Multiwall Carbon Nanotube Bulk Materials. KEQUIN YANG, Clemson University, JIAN HE, ZHE SHU, APPARAO RAO, DEPARTMENT OF PHYSICS AND ASTRONOMY; COMSET, CLEMSON UNIVERSITY, CLEMSON, SC, 29634. — Millimeter long vertically oriented multiwall carbon nanotube (MWNT) arrays with typical tube diameter around 30-50 nm were grown on Si substrates using thermal chemical vapor deposition. The arrays were realigned and densified using a spark plasma sintering process to form oriented MWNT bulk samples. Electron microscopy studies on the as-prepared bulk samples corroborate that the MWNTs are fairly well aligned and the pristine tubular morphology of the MWNTs is preserved during the sintering. The temperature dependent electronic, thermal power and thermal conductivity measurements were performed along different directions relative to the preferred orientation of MWNTs. In particular, the longitudinal and transverse thermal conductivity at 300 K are found to be about 35 W/(mK) and 1 W/(mK), respectively. In the temperature regime between 10 – 300 K, the electrical resistivity is on the order of few mΩcm and exhibits a thermal excitation type temperature dependence, while the Seebeck coefficient is on the order of few μV/K and exhibits a weak temperature dependence. These results give new insights into the unique electrical and thermal transport mechanisms in and between MWNTs.

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11:15AM B37.00001 Phase-Space Explorations in Time-Dependent Density Functional Theory. NEEPA MAITRA, Hunter College and the Graduate Center of the City University of New York — Time-Dependent Density Functional Theory is increasingly popular for calculating excitation and response properties of atoms, molecules, clusters and solids. It has achieved an unprecedented balance between accuracy and efficiency for a wide range of systems, but not all. Although not limited to the linear response regime, there are particular challenges for applications to strong-field processes; for example obtaining momentum distributions, certain electronic quantum control problems, and including memory-dependence necessary in the functional dependence. In this talk we will discuss some of these, and introduce a new extension of the theory where the basic variable is the phase-space density W(r,p,t) (that contains information on both the co-ordinate- and momentum distributions of the electrons), instead of the usual co-ordinate space density n(r,t), to deal with these challenges.

11:51AM B37.00002 Time-dependent density-functional theory for electronic excitations in materials. CARSTEN A. ULLRICH, University of Missouri — There is currently an intense effort underway to study the optical properties of bulk and nanostructured materials using time-dependent density-functional theory (TDDFT). This talk will discuss challenges and recent advances of TDDFT in this area, and present some new applications to excitonic effects in bulk insulators and to collective charge- and spin-density excitations in doped quantum wells. A TDDFT version of the semiconductor Bloch equations is presented, which describes ultrafast electron dynamics, including excitonic effects, in insulators and semiconductors. From this, an excitonic Wannier equation is derived featuring a nonlocal effective electron-hole interaction determined by long-range exchange-correlation effects. Excitonic binding energies are calculated for several direct-gap insulators. The spin Coulomb drag (SCD), which constitutes an intrinsic source of dissipation for spin currents in metals and semiconductors, originates as a dynamical exchange-correlation effect in time-dependent current-DFT. We develop a linear-response description of collective spin-density excitations in quantum wells including SCD as well as Rashba and Dresselhaus spin-orbit coupling, and show that spin plasmon line widths in quantum wells allow a purely optical, quantitative measurement of the SCD effect.

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1Funded by NSF and Research Corporation

2DRI-07 WMR-10
recently developed an efficient many-pole model of the GW self-energy based calculations of dielectric response using a real-space Green’s function approach. The model is applied a posteriori to Kohn-Sham calculations of excited state spectra using a convolution of the spectrum with an energy dependent Lorentzian. The method is found to be widely applicable over a broad range of energies, with little computational cost. Several illustrative examples are presented which show improved agreement between theoretical calculations and experiment for both optical and x-ray spectra.

1 Supported by NIH NCRR BTP grant RR-01209 (JK) and DOE Grant DE-FG02-97ER45623 (JJR and MP).


1 Work supported by DOE ScIADAC grant DE-FC02-06ER25794.

12:51PM B37.00005 Tailoring High-Order Harmonics: A Computational Approach Based on Time-Dependent Density-Functional Theory. ALBERTO CASTRO, DEPARTMENT OF PHYSICS, FREE UNIVERSITY OF BERLIN, ALI AKBARI, ANGEL RUBIO, Universidad del Pais Vasco, EBERHARD GROSS, Department of Physics, Free University of Berlin — Atoms and molecules react in complex manners when they are irradiated with high-intensity electromagnetic pulses: multi-photon, tunneling and over-the-barrier ionisation, laser driven photo-induced isomerisations or fragmentations, and high harmonic generation are some of the non-linear effects that are observed. The so-called pulse shaping techniques can be used to design pulses that produce a desired effect. A technologically appealing possibility is to tailor the harmonic emission spectrum: enhancement of some given orders, supression of others, etc. We have undertaken the task of exploring this possibility from a theoretical point of view, by making use of time-dependent density-functional theory to describe the electrons, a real-space numerical representation, and various optimization techniques.

1:03PM B37.00006 Ab initio calculations of optical spectra by solving the Bethe-Salpeter equation without empty states. Work1, DARIO ROCCA, DEYU LU, GIULIA GALLI, University of California, Davis — We present a novel first principle approach to solve the Bethe-Salpeter equation (BSE) that builds on recent progress in time-dependent density functional perturbation theory [1], and uses an eigenvalue decomposition representation of the dielectric matrix [2]. This approach does not require the explicit calculation of excited single particle electronic states, making it suitable for calculations involving large basis sets and/or a large number of transitions. The numerical solution of the BSE is obtained through a generalized, non-Hermitian Lanczos iterative algorithm and does not require the use of the Tamm-Dancoff approximation. Furthermore, since Lanczos coefficients are frequency independent, optical spectra may be obtained in a very broad energy range. The efficiency and accuracy of the new approach are demonstrated by calculating the optical properties of silicon nanoclusters with up to 1 nm diameter. [1] D. Rocca, R. Gebauer, Y Saad, and S. Baroni, J. Chem. Phys. 128, 154105 (2008). [2] H.Wilson, F.Gygi and G.Galli, Phys. Rev. B, 78:113303 (2008).

1 Work supported by NSF grant CHE-0802907.

1:15PM B37.00007 Time-dependent transition densities2, YONGHUI LI, CARSTEN A. ULLRICH, University of Missouri — To visualize and interpret the induced charges and electron-hole coherences of electronic excitations in molecules, a real-space density matrix analysis is a useful computational tool. We extend this technique into the nonlinear, real-time domain and define the time-dependent transition densities in the context of time-dependent density-functional theory. This opens up the possibility of a real-time monitoring of the optical excitation dynamics in molecules, providing a visualization tool for processes such as exciton migration or charge-transfer excitations. The method will be illustrated for simple one-dimensional model systems.

2 Supported by Research Corporation and NSF DMR-0553485.

12:27PM B37.00008 Is the Kohn-Sham Oscillator Strength Exact at the Ionization Threshold?1, ZENGHUI YANG, University of California, Irvine, CA 92697, USA, META VAN FAASSEN, Afdeling Theoretische Chemie, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, Kingdom of the Netherlands, KIERON BURKE, University of California, Irvine, CA 92697, USA — It is well-established that the highest occupied orbital of the exact Kohn-Sham potential of any system is at -\epsilon, where \epsilon is the ionization energy. Therefore, in optical response, the non-interacting Kohn-Sham electrons in the ground-state potential have a first ionization threshold that exactly matches that of the real system[1]. We show that corresponding the Kohn-Sham oscillator strength is not exact at the first ionization threshold by explicit demonstration for the helium atom. We use a simple fit of the entire photoabsorption spectrum of both the Kohn-Sham potential for helium and that of real helium. We use oscillator strength sum rules[2] to determine the fit parameters, so this fit should be generally useful. [1] M. A. L. Marques, C. A. Ullrich, F. Nogueira, et al. Time-Dependent Density Functional Theory. Springer-Verlag, Berlin, 2006 [2] U. Fano and J. W. Cooper. Rev. Mod. Phys., 40(3), 441-507, 1968

1 This work is funded by U.S. National Science Foundation(Grant No.CHE-0809859)
In density functional theory (DFT), the exchange-correlation functional \( E_{\text{XC}} \) can be exactly expressed by the adiabatic connection integral \([1,2]\). The integrand should satisfy several exact conditions \([3]\). We show that for the low-density limit (as \( \lambda \to \infty \)), the \( \lambda^{-2} \) term in the expansion of the integrand \( W(\lambda) \) should vanish. We propose a simple parametric form for \( W(\lambda) \), satisfying the new exact condition. We apply this interpolation form to Hooke’s atom and helium atom and show that it is accurate for weakly-correlated two-electron systems.

1. 1:39PM B37.00009 An Exact Condition for the Integrand of Adiabatic Connection
ZHENFEI LIU, KIERN BURKE, University of California, Irvine — In density functional theory (DFT), the exchange-correlation functional \( E_{\text{XC}} \) can be exactly expressed by the adiabatic connection integral \([1,2]\). The integrand should satisfy several exact conditions \([3]\). We show that for the low-density limit (as \( \lambda \to \infty \)), the \( \lambda^{-2} \) term in the expansion of the integrand \( W(\lambda) \) should vanish. We propose a simple parametric form for \( W(\lambda) \), satisfying the new exact condition. We apply this interpolation form to Hooke’s atom and helium atom and show that it is accurate for weakly-correlated two-electron systems.

1. 1:51PM B37.00010 New exact and approximate forms for the Luttinger-Ward correlation energy functional within the GW-RPA approximation
SOHRAB ISMAIL-BEIGI, Department of Applied Physics and Center for Research on Interface Structures and Phenomena (CRISP), Yale University — In principle, many-body Green’s function approaches to electronic systems such as the Luttinger-Ward formalism allow one to compute both total energies and quasiparticle excitation spectra (i.e. band structures) simultaneously from first principles. We report on two new results that reformulate the Luttinger-Ward correlation energy functional within the GW-RPA approximation. A first expression is exact and allows for systematic and straightforward evaluation of correlation energies. The second expression is approximate but yields a family of computationally efficient approximations to the correlation energy and the self-energy operator of which the well known Coulomb-hole and screened-exchange (COHSEX) approximation is the lowest order.

2. 2:03PM B37.00011 Non-empirical hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound
MARIANA M. ODASHIMA, KLAUS CAPELLE, Universidade de Sao Paulo — A simple and completely general representation of the exact exchange-correlation functional of density-functional theory is derived from the universal Lieb-Oxford bound for Coulomb-interacting systems. This representation leads to an alternative point of view on popular hybrid functionals. A similar representation of the exact correlation functional allows to construct a family of non-empirical hyper-generalized-gradient approximations (HGGAs), departing from established paradigms of functional construction. Numerical tests and applications of these HGGAs to atoms and molecules demonstrate that even simple Lieb-Oxford based HGGAs are competitive with correlation functionals currently used in solid-state physics and quantum chemistry.

Session B38 DCP: Focus Session: The Chemical Physics of Biological and Biologically-inspired Solar Energy Harvesting II 410

11:15AM B38.00001 Coherence and Decoherence in the Excited States of Light Harvesting Complexes
ROBERT J. SILBEY, Massachusetts Institute of Technology — No abstract available.

11:51AM B38.00002 Electronic coherence in electronic energy transfer despite fast dephasing
GREGORY SCHOLES, University of Toronto — Förster resonance energy transfer (FRET) is a common and fundamental photophysical process in life and materials sciences. FRET is an interchromophore relaxation process that transmits the electronic exciton from an initially excited donor to a ground state acceptor chromophore (light-absorbing molecule). FRET is used, for example, to harvest light in photosynthesis, measure distances in proteins, and it accelerates the photodegradation of polymers. In recent years attention has turned to the study of FRET in complex assemblies of molecules. While Förster theory has enabled the efficiency of FRET to be predicted and analyzed in numerous and diverse areas of study, recent work has aimed to discover ways beyond the Förster mechanism by which electronic energy can be transferred. The talk will compare and contrast theoretical and experimental studies of excitation relaxation in photosynthetic antenna systems with the conjugated polymer poly[2-methoxy,5-(2’-ethyl-hexoxy)-1,4-phenylenevinylene] (MEH-PPV). I will report new work where we have used a new anisotropy experiment to examine coherent energy transfer and a complementary technique using two-dimensional electronic spectroscopy expose the role of coherence transfer in the fastest time dynamics. We find that coherent energy transfer occurs for many tens of femtoseconds, even at room temperature. That leads us to examine the nature and implications of the so-called intermediate coupling regime for EET.

12:27PM B38.00003 Photosynthetic nanoparticle complexes
ALEXANDER GOVOROV, Ohio University — We investigate structures composed of a photosynthetic molecule and a semiconductor (metal) nanoparticle \([1]\). The rate of optical generation of electron-hole pairs inside a photosynthetic system can be greatly increased through conjugation with nanoparticles. In the case of a semiconductor nanoparticle, the enhancement effect comes from the essentially larger optical absorption cross-section of a semiconductor nanoparticle compared to a photosynthetic system. In this hybrid complex, excitons are transferred via the Förster mechanism to the photosynthetic system, where charge separation takes place. For metal nanoparticles conjugated with a photosynthetic system, we predicted a strong enhancement effect due to the plasmon resonance. Such an enhancement effect was recently observed at Munich U. \([2]\). In summary, we have shown that one can use crystalline nanoparticles to create a 10-fold enhancement of the initial stage of photosynthesis, i.e. the absorption process. Potential applications of nanocrystal complexes are in light-harvesting. \([1]\) A. O. Govorov and I. Carmeli, Nano Lett. 7, 620 (2007); \[2\] S. Mackowski, S. Wörnke, A.J. Maier, T.H.P. Brosotudarmo, H. Harutyunyan, A. Hartschuh, A.O. Govorov, H. Scheer, C. Bräuchle, Nano Lett. 8, 558 (2008).

1. Supported by NSF and Air Force Research Labs
12:39PM B38.00004 Quantum coherence, decoherence and entanglement in light harvesting complexes, MARTIN PLENIO, FILIPPO CARUSO, Imperial College London, ALEX CHIN, University of Hertfordshire, ANIMESH DATTA, Imperial College London, SUSANA HUELGA, University of Hertfordshire — Transport phenomena in networks allow for information and energy to be exchanged between individual constituents of communication systems, networks or light-harvesting complexes. Environmental noise is generally expected to hinder transport. Here we show that transport of excitations across dissipative quantum networks can be enhanced by dephasing noise. We identify two key processes that underly this phenomenon and provide instructive examples of quantum networks for each. We argue that Nature may be routinely exploiting this effect by showing that exciton transport in light harvesting complexes and other networks benefits from noise and is remarkably robust against static disorder. These results point towards the possibility for designing optimized structures for transport, for example in artificial nano-structures, assisted by noise. Furthermore, we demonstrate that quantum entanglement may be present for short times in light-harvesting complexes. We describe how the presence of such entanglement may be verified without the need for full state tomography and with minimal model assumptions. This work is based on M.B. Plenio & S.F. Huelga, New J. Phys. 10, 113019 (2008) and F. Caruso, A. Chin, A. Datta, S.F. Huelga & M.B. Plenio, in preparation.

12:51PM B38.00005 Non-radiative decay processes in InAs nanocrystals, MARCO CALIFANO, University of Leeds — The mechanisms governing excited state relaxation in semiconductor nanocrystals (NCs) are still not well understood. The validity of the Auger electron cooling and multiexciton recombination hypotheses, which would explain much of the experimental data available to date, has recently been questioned. Moreover the recent observation of sub-picosecond electron relaxation times and bimolecular recombination rates of the order of 0.1-1 ps in InAs, although qualitatively ascribed to Auger processes, still awaits a quantitative theoretical interpretation. Multiexciton recombination is particularly important as its signatures are used to detect and quantify carrier multiplication efficiency in NCs. Furthermore efficient non-radiative (multi-)exciton decay represents a major obstacle for application of NCs in lasing and photovoltaics. A quantitative theoretical understanding of these processes is therefore critical for any technological implementation of quantum-dot-based devices. The results of a detailed investigation using the pseudopotential method provide an explanation of the observed lifetimes in terms of Auger-like decay mechanisms, supporting the Auger interpretation of excited state relaxation in NCs.

1 Supported by NREL's LDRD program.

1:03PM B38.00006 Exciton Transport Simulations in Phenyl Cored Thiophene Dendrimers, KWISEON KIM, MUHAMMET ERKAN KOSE, PETER GRÅF, NIKOS KOPIDAKIS, GARRY RUMBLES, National Renewable Energy Laboratory, SEAN E. SHAHEEN, University of Denver — Phenyl cored 3-arm and 4-arm thiophene dendrimers are promising materials for use in photovoltaic devices. It is important to understand the energy transfer mechanism in these molecules to gain insight into the synthesis of novel dendrimers with improved efficiency. A method is developed to estimate the exciton diffusion lengths for the dendrimers and similar chromophores in amorphous films. The approach exploits Fermi's Golden Rule to estimate the energy transfer rates for an ensemble of bimolecular complexes in random orientations. Using Poisson's equation to evaluate Coulomb integrals, we are led to efficient calculation of excitonic couplings between the transition densities. Monte-Carlo simulations revealed the dynamics of energy transport in the dendrimers. Experimental exciton diffusion lengths of the dendrimers range 10-20 nm, increasing with the size of the dendrimer. Simulated diffusion lengths correlate well with experiments. The chemical structure of the chromophore, the shape of the transition densities and the exciton lifetime are found to be the most important factors that determine the exciton diffusion length in amorphous films.

1:15PM B38.00007 Efficient and Long-lived Charge Separation in a Heteroleptic Ruthenium(II) Polypyridyl Complex, JOSEPH HENRICH, HAOYU ZHANG, JEREMY WHITE, PRABIR DUTTA, BERN KOHLER, The Ohio State University — The excited-state dynamics of a tris-bidentate mononuclear ruthenium(II) complex, [(bpy)2RuL4]3+ (where bpy = bipyridine, L4-DQ = 1-[4-(4'-methyl)-2,2'-bipyridyl]) was investigated by femtosecond transient absorption spectroscopy in bulk solution and tethered to a zeolite nanocrystal. [(bpy)2RuL4]3+ is a promising photosensitizer molecule for artificial photosynthesis. Broadband transient absorption experiments in bulk acetone and liquid helium matrices revealed that excitation of the MLCT absorption band transfers an electron within one picosecond from the metal center to the bipyridinium (DQ) ligand. Back electron transfer then takes place with a time constant of 1.45 ns. Highly efficient charge separation is attributed to the conjugated nature of the bipyridinium-terminated ligand. When [(bpy)2RuL4]3+ is tethered to a zeolite Y particle, charge can be transferred to a methyl viologen molecule encapsulated in the zeolite. Zeolites are promising materials for solar energy conversion because of their ability to slow rates of charge recombination. The effects of the zeolite on the photoprocesses of the ruthenium polypyridyl complex will be presented.

1:27PM B38.00008 First-Principles Studies of Single-Molecule Photovoltaics, PETER DOAK, UC Berkeley Chemistry, R. A. SEGALMAN, UC Berkeley Chemical Engineering, T. D. TILLEY, UC Berkeley Chemistry, J. B. NEATON, LBNL Molecular Foundry — Organic photovoltaics consist of electron donor and acceptor polymers or molecules blended together, and are promising inexpensive, lightweight alternatives to conventional silicon solar cells. However, many of the physical processes responsible for their poor efficiencies are not well understood. Here, using first-principles calculations based on density functional theory, including self-energy corrections within the GW approximation and a discussion of excitonic effects, we examine the relationship between molecular structure and electronic level alignment at a covalent donor-acceptor interface. We consider small asymmetric molecules subdivided into discrete covalently linked moieties based on thiophene, tetrafluorobenzene, pyridine, and durene. Excited states of each of these moieties, as well as their covalently-linked combinations, are computed and discussed in the context of their ability to absorb photons and separate charge. Work supported in part by the DOE Helios SERC. Computational resources provided by NERSC.

1:39PM B38.00009 Intramolecular Interactions in Novel Macrocyclic Materials, THEODORE GOODSON, University of Michigan — In this presentation I will report a strongly interacting new dendrimer system with an extended spectroscopic unit (coherent domain) beyond the trimer configuration. Strong cooperative enhancement of two-photon absorption cross-section was observed when going from the trimer arrangement to the next generation. Combination of a variety of femtosecond spectroscopy methods such as femtosecond time-resolved fluorescence upconversion, transient absorption, transient grating, three pulse photon echo peak shift experiments complemented with those of steady state spectroscopy allowed us to compare the properties of absorption states with those of fluorescence states, to estimate the reorganization energies, and the extent of inhomogeneous broadening. Our measurements indicated that spectroscopic units in this dendrimer are different for the trimer system and for the dendrimers of higher generation numbers. This coherent domain extends over the trimer geometry and its size is comparable with the size of the dendrimer G1 comprising nine linear segments. We have also investigated the novel applications of a two-dimensional carbon network structure's building blocks. The material shows very interesting two-photon absorption properties as well as strongly coupled optical excitations. They have also been suggested as good building blocks for molecular electronics applications.
The force-velocity relation of growing actin filaments. A simple model based on entropic forces seems to explain our observations. Protrusions at the cell surface and leads to cell motility. Using magnetic colloids, we measure how the chemical reaction of polymerization generates mechanical interactions.

CARLIER, JEROME BIBETTE, LCMD, ESPCI TEAM, PMMH, ESPCI TEAM, LEBS, CNRS TEAM, NYU PHYSICS TEAM — Actin polymerization drives study cytoskeletal dynamics during the spreading process. Actin filaments spontaneously organized into a variety of structures including traveling waves, target reflection contrast microscopy. We found that the spread area exhibited a sigmoidal growth as a function of time in contrast to the previously proposed universal contribution to the processes involved in the interaction with the substrate, such as the elastic response and adhesion.

A single cell and put it in contact with an adhesive surface mounted on a translation stage. The spring constant of the micropipette is carefully measured and its mechanical contributions of intercellular junctions and focal adhesions while also providing insight into the important materials properties and length scales that govern cell sheet responses.

11:27AM B39.00002 Locomotion of C. elegans through jammed granular media, KEVIN LU, PAULO E. ARRATIA, University of Pennsylvania — It is quantitatively demonstrated in this experiment on the undulatory swimming of C. (Caenorhabditis) elegans that, in a highly-resistive media, the animal only executes beating frequencies and amplitudes in discrete values. This behavior of C. elegans is inferred from the peaks in the particle velocity distributions where the most probable velocities match the transverse velocities of the nematode body. The behavior in the velocity distribution is more pronounced for particles in denser arrangements and for those closer to the thrashing gait of the worm. These results contribute to the existing data on the worm locomotion and further facilitate the identification of the endogenous genes and neural circuitry to the exogenous behavioral responses of C. elegans.

11:39AM B39.00003 Mechanics of an Ultrafast Cellular Contraction, GAURAV MISRA, RICHARD B. DICKINSON, TONY LADD, University of Florida — Vorticella Convallaria is one of a class of fast-moving organisms, traversing its body size in less than a millisecond. It has two main parts, the cell body and a stalk, which attaches the cell body to the substrate. The stalk houses a slender, elastic structure called Spasmoneme, which winds helically inside the stalk and generates a strong tensile force in response to Calcium signaling. We are developing numerical simulations of the collapsing stalk to quantify the magnitude and time scale of the force generation. We have coupled a Kirchhoff model of an elastic rod (representing the stalk) with an embedded helically wound filament (representing the Spasmoneme). Contraction of this assembly is driven by a constant velocity Calcium signal that induces a state of tension in the Spasmoneme. Depending on the speed of the Calcium signal, we observe different mechanical responses from the contracting stalk, which we compare with experimental observations. We follow the interplay of contraction, twist and bend to explain some unexpected features of the retraction process. Two different macroscopic models have been proposed to explain the time-dependent velocity of the cell body; we compare the predictions of these models with the dynamics revealed by our filament model.

11:51AM B39.00004 Polymer Microlenses for Quantifying Cell Sheet Mechanics, GUILLAUME MIQUELARD-GARNIER, University of Massachusetts Amherst, JESSICA ZIMBERLIN, PATRICIA WADSWORTH, ALFRED CROSBY — Mechanical interactions between individual cells and their substrate have been studied extensively over the past decade; however, our understanding of how these interactions change as cells interact with neighboring cells in the development of a cell sheet, or early stage tissue, is less developed. We present a recently developed experimental technique for quantifying the mechanics of confluent cell sheets (Zimberlin J.A., et al., Cell Motility and the Cytoskeleton, 65, 9, 762). Living cells are cultured on a thin film of polystyrene [PS], which is attached to a patterned substrate of crosslinked poly(dimethyl siloxane) microwells. As the cell sheet grows, cells apply sufficient force to buckle the PS film over individual microwells to form a microlens array. The curvature for each microlens is measured by confocal microscopy and can be related to the strain and stress applied by the cell sheet. We demonstrate that this technique can be used to decouple mechanical contributions of intercellular junctions and focal adhesions while also providing insight into the important materials properties and length scales that govern cell sheet responses.

12:03PM B39.00005 Why is Actin Patchy?, ANDERS CARLSSON, Washington University in St. Louis — The intracellular protein actin, by reversibly polymerizing into filaments, generates forces for motion and shape changes of many types of biological cells. Fluorescence imaging studies show that actin often occurs in the form of localized patches of size roughly one micrometer at the cell membrane. Patch formation is most prevalent when the free-actin concentration is low. I investigate possible mechanisms for the formation of actin patches by numerically simulating the “dendritic nucleation” model of actin network growth. The simulations include filament growth, capping, branching, severing, and debranching. The attachment of membrane-bound activators to actin filaments, and subsequent membrane diffusion of unattached activators, are also included. It is found that as the actin concentration increases from zero, the actin occurs in patches at lower actin concentrations, and the size of the patches increases with increasing actin concentration. At a critical value of the actin concentration, the system undergoes a transition to complete coverage. The results are interpreted within the framework of reaction-diffusion equations in two dimensions.

1 Supported by the National Institutes of Health under Grant R01-GM086882.

12:15PM B39.00006 Direct dynamical measurement of the cytoskeletal contribution to the adhesion and mechanics of living cells, MARIE-JOSEE COLEBRT, CECILE FRADIN, KARI DALNOKI-VERESS, Department of Physics and Astronomy, McMaster University — The cytoskeleton is involved in the interaction of the cell with its surroundings through adhesion and the elastic response of the cell. To dynamically probe these properties, we have developed a new tool that takes advantage of an ‘L’-shaped micropipette to micromanipulate a single cell and put it in contact with an adhesive surface mounted on a translation stage. The spring constant of the micropipette is carefully measured and its deflection is used to apply a calibrated force. This technique gives access to real time monitoring of the cell response to an applied deformation, thus exploring the relaxation processes of the cell when subjected to an external load. The polymerization of actin and microtubules is prevented to explore the cytoskeletal contribution to the processes involved in the interaction with the substrate, such as the elastic response and adhesion.

12:27PM B39.00007 Force generated by polymerization of actin filaments: an entropic role?, JEAN BAUDRY, CORALINE BRANGBOUR, OLIVIA DU ROURE, EMMANUELE HELFER, MARC FERMIGIER, PAUL M. CHAIKIN, MARIE-FRANCE CARLIER, JEROME BIBETTE, LCMD, ESPCI TEAM, PMMH, ESPCI TEAM, LEBS, CNRS TEAM, NYU PHYSICS TEAM — Actin polymerization drives protrusions at the cell surface and leads to cell motility. Using magnetic colloids, we measure how the chemical reaction of polymerization generates mechanical forces. Rapid force-distance measurement gives us access to the forces that control the migration of colloids, whereas long experiments at constant forces give the force-velocity relation of growing actin filaments. A simple model based on entropic forces seems to explain our observations.

12:39PM B39.00008 Cytoskeleton mediated spreading dynamics of immune cells, KING-LAM HUI, JESSICA WANT, BRIAN GROOMAN, ARPITA UPADHYAYA, Department of Physics, University of Maryland — We have studied the spreading of Jurkat T-cells on anti-CD3 antibody-coated substrates as a model of immune synapse formation. Cell adhesion area versus time was measured via interference reflection contrast microscopy. We found that the spread area exhibited a sigmoidal growth as a function of time in contrast to the previously proposed universal power-law growth for spreading cells. We used high-resolution total internal reflection fluorescence microscopy of these cells transfected with GFP-actin to study cytoskeletal dynamics during the spreading process. Actin filaments spontaneously organized into a variety of structures including traveling waves, target patterns, and mobile clusters emanating from an organizing center. We quantify these dynamic structures and relate them to the spreading rates. We propose that the spreading kinetics are determined by active rearrangements of the cytoskeleton initiated by signaling events upon antibody binding to T-cell receptors. Membrane deformations induced by such wave-like organization of the cytoskeleton may be a general phenomenon that underlies cell movement and cell-substrate interactions.
12:51PM B39.00009 How deep cells feel: Mean-field Computations and Experiments, AMNON BUXBOIM, SHAMIK SEN, University of Philadelphia, DENNIS E. DISCHER1 — Most cells in solid tissues exert contractile forces that mechanically couple them to elastic surroundings and that significantly influence cell adhesion, cytoskeletal organization and differentiation. However, strains within the depth of matrices are often unclear and are likely relevant to thin matrices, such as basement membranes, relative to cell size as well as to defining how far cells can "feel." We present experimental results for cell spreading on thin, ligand-coated gels and for prestress in stem cells in relation to gel stiffness. Matrix thickness affects cell spread area, focal adhesions and cytoskeleton organization in stem cells, which we will compare to differentiated cells. We introduce a finite element computation to estimate the elastic deformations within the matrix on which a cell is placed. Interfacial strains between cell and matrix show large deviations when soft matrices are a fraction of cell dimensions, proving consistent with experiments. 3-D cell morphologies that model stem cell derived neurons, myoblasts, and osteoblasts show that a cylinder-shaped myoblast induces the highest strains, consistent with the prominent contractility of muscle. Groups of such cells show weak crosslink via matrix strains only when cells are much closer than a cell-width. Cells thus feel on length scales closer to that of adhesions than on cellular scales.

1University of Philadelphia

1:03PM B39.00010 Tether extrusion from biomimetic cells, KARINE GUEVORKIAN, LÉA LAETITIA PONTANI, CÉCILE SYKES, FRANÇOISE BROCHARD-WYART, Institut Curie — The plasma membrane of a cell is coupled to its underlying cytoskeleton through membrane binding proteins. By pulling membrane tethers, one can measure the strength of these attachments and also probe the rheology of the membrane. In the past, we have used the hydrodynamic tether extrusion technique to study tether dynamics of Red Blood Cells [1]. To describe the non-linear force-velocity behavior at high extrusion forces, we have developed a theoretical model based on lipid permeation through the network of membrane binding proteins [2]. To test this model, we use a biomimetic system consisting of liposomes encapsulating an actin cortex in which the density of membrane-cytoskeleton linkers can be controlled. Here we will present our recent experimental results and compare them to the theoretical predictions. [1] N. Borghi et al, Biophys. J. 93 (2007) [2] F. Brochard-Wyart, et al, Proc. Natl. Acad. Sci. USA, 103 (2006)

1:15PM B39.00011 Mechanics of Nascent Cell Adhesions, CÉCILE O. MEJEAN, ANDREW W. SCHAFFER, PAUL FORSCHER, ERIC R. DUFRESNE, Yale University — Cells have the ability to sense and respond to mechanical and biochemical cues from their environment. In neurons, the binding and restraint of transmembrane cell adhesion molecules (CAMs) can trigger acute periods of axon growth. Preceding growth, the cell must create a stiff mechanical linkage between the CAM and the cytoskeleton. Using holographic optical tweezers, we manipulate CAM-coated beads on the membrane of the cell. We investigate the dynamics of the mechanical properties of this linkage as a function of time, applied force, and CAM density. We find that CAM-coated beads exhibit stochastic intermittent binding to the cytoskeleton. In time, we observed that the adhesions stiffen and their mechanical properties depend on the applied force. Treatment of cells with small molecules that alter cytoskeletal dynamics are used to probe the roles of actin filament assembly and myosin motor activity in adhesion formation.

1:27PM B39.00012 Epithelial Mechanics during Germband Retraction in Fruit Fly Embryogenesis, XIAOYAN MA, HOLLEY E. LYNCH, M. SHANE HUTSON, Dept. of Physics & Astronomy, Vanderbilt University — During germ-band retraction in the early embryonic development of fruit fly embryos, the epithelial cells of the amnioserosa (AS) undergo a dramatic change in cell shape. The average cell aspect ratio reduces from \(\alpha \sim 10\) to \(\sim 1\) within three hours. We performed laser hole-drilling and confocal microscopy to investigate the mechanics of this process in live fly embryos. We find that the laser-induced recoil dynamics of AS cells during germ-band retraction (when \(\alpha \sim 10\)) is dramatically different from that during the later dorsal closure stage (when \(\alpha \sim 1\)). First, in the earliest stage of germband retraction, some AS cells actually shrink instead of expand in the first one second after ablation. After this point, the cells do slowly expand. Second, in either phase, the cell speeds were much slower, in the range of \(\pm 1 \mu m/second\) (compared with speeds in excess of \(10 \mu m/second\) during dorsal closure). Theses results suggest a much smaller tensile mood (and in some cases, compressive) stress in the whole cell sheet in early germband retraction. As retraction proceeds towards dorsal closure, the stresses increase.

1:39PM B39.00013 Matrix elasticity directs stem cell differentiation in 3D too, ALLISON ZAJAC, FLORIAN REHFELDT, DENNIS DISCHER, University of Pennsylvania — Microenvironments appear important in stem cell lineage specification but can be difficult to adequately characterize or control with soft tissues. Naive mesenchymal stem cells (MSCs) are shown here to specify lineage andcommit to phenotypes with extreme sensitivity to tissue level elasticity. Soft matrices that mimic brain microenvironment are more sensitive, stiffer matrices that mimic muscle microenvironment, and comparatively rigid matrices that mimic collagenous bone prove osteogenic. During the initial week in culture, reprogramming of these lineages is possible with addition of soluble induction factors, but after several weeks in culture, the cells commit to the lineage specified by matrix elasticity, consistent with the elasticity-insensitive commitment of differentiated cell types. Inhibition of nonmuscle myosin II blocks all elasticity-directed lineage specification—without strongly perturbing many other aspects of cell function and shape. The results have significant implications for understanding physical effects of the in vivo microenvironment and also for therapeutic uses of stem cells.

1:51PM B39.00014 Cell response to long term mechanical interaction with nanopipettes, ZULFIYA ORYNBAYEVA, Drexel University, RIJU SINGHAL, ELINA VITÖL, MICHAEL BOUCHARD, JANE AZIZKHAN-CLIFFORD, BRADLEY LAYTON, GARY FRIEDMAN, YURY GOGOTSI, KECK INSTITUTE FOR ATTOFLUIDIC NANOTUBE-BASED PROBES TEAM — Traditional microinjection into cells is performed over a relatively short term. Pipettes are typically withdrawn following any kind of injection. On the other hand, there is growing interest in using nanopipettes for cellular and subcellular probing. This interest is partly due to new developments in nanopipette technology which employ carbon nanotubes and provide robustness, flexibility, and biocompatibility. However, as far as we know, no systematic study of physiological, biochemical, and biophysical processes associated with cell response to lengthy mechanical stimulations by nanopipette probing have been performed so far. We present a detailed investigation of a wide range of effects of long term pipette insertion into a cell. Both traditional glass micropipettes and the novel carbon nanotube-tipped probes were involved in this study. The mechanism of Ca2+ response to the mechanical stimuli introduced by the nanopipette, and the role of different organelles in this mechanism were studied. We hypothesize that the calcium response is a function of cytoskeleton integrity and the mode of coupling between the cytoskeleton and the plasma membrane domains.

2:03PM B39.00015 Gold Nanoparticles effect on Human Dermal Fibroblast, TATSIANA MIRONAVA, NADINE PERNOLET, MIRIAM RAFAILOVICH, SUNY at Stony Brook, MATERIAL SCIENCE AND ENGINEERING DEPARTMENT TEAM — Recently many researchers brought to the light the fact that due to high surface/bulk ratio nanoparticles can penetrate unusually deep human organs and cause health problems. Gold nanoparticles are widely used nowadays, however, their effects on cells are still under investigation. Here, we studied the effect of inert citrate/gold nanoparticles as a function of size (13 nm and 45 nm), concentration and time exposure (from 1 to 6 days) on human dermal fibroblasts, since skin is one of the major routes to exposure to nanoparticles. We measured apoptosis rate as a function of nanoparticles size, time exposure and concentration. We found that the presence of 45-nm gold particles had more severe effects on these cells when compared to 13-nm nanoparticles, as the nanoparticles entry use 2 different pathways. In addition the question of cells recovery as a function of time exposure and concentration was investigated.

11:15AM  B40.00001  Amino Acid Free Energy Decomposition  . HUI WANG, MICHAEL FAIRCILD, DENNIS LIVESAY, DONALD JACOBS, University of North Carolina at Charlotte — The Distance Constraint Model (DCM) describes protein thermodynamics at a coarse-grained level based on a Free Energy Decomposition (FED) that assigns energy and entropy contributions to specific molecular interactions. Application of constraint theory accounts for non-additivity in conformational entropy so that the total free energy of a system can be reconstituted from all its molecular parts. In prior work, a minimal DCM utilized a simple FED involving temperature-independent parameters indiscriminately applied to all residues. Here, we describe a residue-specific FED that depends on local conformational states. The FED of an amino acid is constructed by weighting the energy spectra associated with local energy minima in conformational space by absolute entropies estimated using a quasi-harmonic approximation. Interesting temperature-dependent behavior is found. Support is from NIH R01 GM073082 and a CRI postdoctoral Duke research fellowship for H. Wang.

11:27AM  B40.00002  Surface Induced Self-Assembly of Fibrinogen Fibers in the Absence of Thrombin  . JASEUNG KOO, MIRIAM RAFAILOVICH, DENNIS GALANAKIS, Stony Brook University — Wound healing is a complex process imitated by the formation of fibrin fibers that are involved in clot formation and fibrinolysis migration. Normally this process is triggered by thrombin cleavage of the E domain on the fibrinogen molecules, which allows them to spontaneously self-assemble into the fibers. Here we demonstrate that this process can also be initiated in the absence of thrombin. We show that by simply placing the proteins in contact with hydrocarbon functionalized clay surfaces, molecular reorientation occurs which allows fibers to form from the intact fibrinogen protein. Furthermore, using monoclonal antibodies, we determined which regions on the αC domains are involved in the formation of the new fibrinogen fibers. This allowed us to extend these findings to general hydrophobic surfaces, such as those presented by most hydrocarbon polymers. On the other hand, the carbonyl terminal part of the Aα chain, can interact with amine containing polymers, and suppress formation of the fibers.

11:39AM  B40.00003  On the Rate and Mechanism of Proton Transfer Reactions in Proteins1 . AIHUA XIE, YUNXING LI, EDWARD MANDA, BEINING NIE, WOUTER HOFF, Oklahoma State University, RICHARD MARTIN, Los Alamos National Lab — One of the fundamental processes in molecular biology is proton transfer reactions in proteins. Proton transfer is essential for the biological functions of proteins responsible in bioenergetics, biological signaling, and enzymatic catalysis. The mechanism of proton transfer is of great interests in order to understand the structural basis of biological functions. Despite of extensive experimental and computational efforts, it remains elusive what a proton to move from the proton donor to the proton acceptor. We will report a proof of concept study regarding a general mechanism of internal proton transfer reactions in proteins. Density functional theory, B3LYP/6-311+G(2d,p), is employed in this study. The results of our study provide deep insights into the structural basis to the rate and mechanism of proton transfer reactions in proteins, such as bacteriorhodopsin and green fluorescence protein.

1This work is supported from Oklahoma Center for the Advancement in Science & Technology and National Science Foundation.

11:51AM  B40.00004  Probing the reversibility of the Dscam Dimer with Light Scattering and Colloids  . JESSE COLLINS, Harvard SEAS; DIETMAR SCHMUCKER, Harvard/Dana Farber Cancer Institute, VINOTHAN MANOHARAN, Harvard — Dscam (Down-syndrome cell adhesion molecule) is a fascinating example of the highly specific interactions unique to biomolecules. The extracellular domain is spliced into over 18,000 isoforms. With few exceptions, each isoform, despite conservation of over 95% of amino acid residues between isoforms, binds to itself and to no other in the set. We investigate the effect of salt and pH on the reversibility of this interaction.

12:03PM  B40.00005  Using Fluorescence Spectroscopy to Evaluate Hill Parameters and Heterogeneity of Ligand Binding to Cytochromes P4501 . GLENN A. MARSCH, BENJAMIN CARLSON, JENNIFER HANSEN, ELAINE MIHELC, Grove City College Physics Department, MARTHA V. MARTIN, F. PETER GUENGERICH, Vanderbilt University School of Medicine — The cytochromes P450 (CYPs) are hemoproteins that oxidize many drugs and carcinogens. Binding interactions of two CYPs with Nile Red, pyrene, and alpha-naphthoflavone were studied using fluorescence quenching. Upon interaction with CYPs, fluorescence from pyrene excited-state dimers was quenched more efficiently than fluorescence from pyrene monomers. Quenching data was fit to the Hill equation to determine binding affinities and the Hill parameter n for the interaction of the substrates with CYPs. All ligands showed strong binding to the CYPs, especially alpha-naphthoflavone, but exhibited little or no cooperativity in the interaction. Modified Stern-Volmer plots were used to confirm binding affinities, and suggested heterogeneous populations of amino acid fluorophores. Fluorescence anisotropy experiments suggest that CYP molecules tumble more rapidly when alpha-naphthoflavone is added.

1We thank the Grove City College Swezey Fund for its support of this project.

12:15PM  B40.00006  UV Resonance Raman Excitation Profiles and Depolarization Ratios of Peptide Conformations  . BHAVYA SHARMA, SANFORD ASHER, University of Pittsburgh — UV resonance Raman spectroscopy is a well established technique for probing peptide and protein secondary structure. Excitation between 180 to 215 nm, within the π to π* electronic transitions of the peptide backbone, results in the enhancement of amide vibrations. We use UVRIR excitation profiles and depolarization ratios to examine the underlying peptide bond electronic transitions. The present consensus is that three electronic transitions (n to π* and two π to π*) occur in simple amides between 230 and 130 nm. In α-helices a weak n to π* electronic transition occurs at 220 nm, while a higher frequency π to π* transition occurs at 190 nm. This π to π* transition undergoes excitation splitting, giving rise to two dipole-allowed transitions: one perpendicular to the helical axis (190 nm) and the second parallel to the axis (205 nm). The melted state of α-helices resembles left-handed poly-proline II (PPII) helices. The PPII helix electronic transitions have been defined as an n to π* transition at ~220 nm and a π to π* transition at ~200 nm. For beta-sheets, the π to π* transition occurs at ~194 nm for parallel and ~196 nm for anti-parallel sheets. n to π* transition occurs at ~217 nm for both.

12:27PM  B40.00007  UV Resonance Raman Spectral Hydrogen Exchange Studies of Poly-L-Lysine’s Conformation  . LU MA, SANFORD ASHER, University of Pittsburgh — The rate of exchange of peptide backbone NH group with the hydrogen of aqueous solvents is sensitive to the peptide secondary structure. In this work, we use a continuous flow rapid mixing technique and study H/D exchange rates of the model peptide poly-L-lysine (PLL) using UV resonance Raman spectroscopy. Different conformational equilibria of PLL between the helical (α, 310, and -helix) and extended conformations (PPII and 2.5,-helix) are obtained by controlling solvent pH and salt concentration. The Amil’ band of the peptide backbone is used as the deuterium marker. The H/D change rate of PLL provides direct information of the stability of different conformations. Additionally, these results provide insight into backbone conformational fluctuations and how various factors affect the conformation.

12:39PM  B40.00008  Polyglycine in Solution, Random or Ordered?  . SERGEI BYKOV, SANFORD ASHER, University of Pittsburgh — According to the existing theories during folding, the protein backbone undergoes a transition from unordered (random coil) to ordered (native) conformations. Understanding the nature of the unordered state is one of the key problems in protein folding. Some recent investigations indicate that unfolded peptides and proteins in solution form structures close to PPII helices. Glycine based peptides possess greater conformational freedom due to the lack of the side chains. This high flexibility makes polyglycine an important model system for investigating of the conformational preferences of the polypeptides backbone in solution in general and for understanding the nature of the unfolded states in particular. We utilized UV Resonance and Visible Raman spectroscopy to investigate conformational preferences of glycine based peptides of different lengths in water solution at different conditions. We will discuss conformational preferences of the glycine based peptides in solution, and define the major factors which govern these conformational preferences.
1:03PM B40.00010 Hydrodynamic and Conformational Properties of Unfolded Proteins. GUY BERRY, Carnegie Mellon University — Published data on the characterization of unfolded proteins in dilute solutions in aqueous guanidine hydrochloride are analyzed to show that the data are not fit by either the random-flight or wormlike chain models for linear chains. The analysis includes data on the intrinsic viscosity, root-mean-square radius of gyration, from small-angle x-ray scattering, and hydrodynamic radius, from the translational diffusion coefficient. It is concluded that residual structure consistent with that deduced from nuclear magnetic resonance on these solutions can explain the dilute solution results in a consistent manner through the presence of ring-structures, which otherwise have an essentially flexible coil conformation. The ring-structures could be in a state of continual flux and rearrangement. Calculation of the radius of gyration for the random-flight model gives a similar reduction of this measure for chains joined at their endpoints, or those containing loop with two dangling ends, each one-fourth the total length of the chain. This relative insensitivity to the details of the ring-structure is taken to support the behavior observed across a range of proteins.

1:15PM B40.00011 Stability versus flexibility in the dimerization kinetics and thermodynamics of the GCN4 Leucine zipper. DIPAK RIMAL, YANXIN LIU, PREM CHAPAGAIN, BERNARD GERSTMAN, Florida International University, THEORETICAL AND COMPUTATIONAL BIOPHYSICS TEAM — We present results of computer simulations that show that too much stability of the native state can have the unwanted side-effect of slower and less reliable folding. The time spent in non-native configurations depends on both the depth of the valleys in the energy landscape and the probability for visiting various regions of the landscape. We present computational results for dimerization of the GCN4 Leucine zipper in which both the helical propensities and the ionic interactions are varied in strength. The results show that when interactions are too strong, they not only beneficially stabilize the native state, but also stabilize non-native configurations that act as kinetic traps. In some cases, intermediate structures become too rigid that the peptide does not have the flexibility necessary to fold to the native state. In other situations, such as high temperature, the chain has superfluous flexibility and can form non-native bonds. If these non-native bonds are too strong, the peptide spends significant time in contorted non-native configurations and folding is slowed and less efficient. Therefore, efficient folding must be a compromise between stability and flexibility.

1:27PM B40.00012 Intermediate states of globular proteins during temperature-induced folding and unfolding studied using small angle x-ray scattering1. JOSE BANUELOS, New Mexico State University, JACOB URQUI'D, New Mexico State University; LANSE; Los Alamos National Laboratory — The ability of proteins to change their conformation in response to changes in their environment has consequences in biological processes like metabolism, chemical regulation in cells, and is believed to play a role in the onset of several neurological diseases such as Alzheimer's disease. The folding process of proteins is characterized by the transition from an randomly coiled state to a compact native conformation. As a protein unfolds, the ratio of nonpolar to polar groups exposed to water changes, affecting a protein’s thermodynamic properties. Using small angle x-ray scattering (SAXS), we are currently studying the intermediate protein conformations that arise during the folding/unfolding process as a function of temperature for a series of globular proteins. The temporal stability of these ensembles is also under investigation. Trends in the scattering profiles, along with correlations with protein thermodynamics, may help elucidate shared characteristics between all proteins in their folding behavior.

2:03PM B40.00015 Generalized distance and its application in protein folding. ALI MOHABZAB, University of British Columbia, STEVE PLOTKIN COLLABORATION — The concept of Euclidean distance between two points can be generalized to extended objects. The generalized distance $D$ can be used as a reaction coordinate in protein folding process. Here $D$ is compared and contrasted with some well-known reaction coordinates, Q and RMSD and is applied to protein fragments such as alpha helix and beta hairpin. The non-crossing constraint in utilizing $D$ is also discussed.

Monday, March 16, 2009 11:15AM - 2:15PM
Session B41 DMP DCMP: Heavy Fermion 115 Superconductors 413
11:15AM B41.00001 Penetration depth study of CeIrIn₃₁, DANIEL VANDERVELDE, Univ. of Illinois, Urbana, H.Q. YUAN, Zhejiang University, Y. ONUKI, Osaka University, M.B. SALAMON, Univ. of Texas at Dallas — The heavy-Fermion compounds CeTIn₅, with T a transition metal, provide a fertile ground for studying the interplay between magnetism and superconductivity. The T = Co compound has a transition temperature Tc = 2.4 K, and has a d-wave order parameter. As Ir is substituted for Co, the transition temperature decreases sharply to Tc = 0.4 K. One report of the thermal conductivity of CeIrIn₃ supports a d-wave state, another argues in favor of a hybrid gap state with broken time-reversal symmetry. We report penetration depth studies of CeIrIn₃ to Tc/5 that supports the d-wave scenario. Converted to superconducting fraction, the data taken with the rf measuring field along various crystallographic axes can be scaled to collapse to a single curve that matches a d-wave calculation with a zero-temperature gap of 2.5kBTc.

1Work supported in part by DOE Grant No. DEFG02-91ER45439.

11:27AM B41.00002 Magnetic-field induced quantum critical points of valence transition in Ce- and Yb-based heavy fermions, SHINJI WATANABE, University of Tokyo, ATSUSHI TSURUTA, KAZUMASA MIYAKE, Osaka University, JACQUES FLOQUET, CEA Grenoble — Valence instability and its critical fluctuations have attracted much attention recently in the heavy-electron systems. Valence fluctuations are essentially charge fluctuations, and it is highly non-trivial how the quantum critical point (QCP) as well as the critical end point is controlled by the magnetic field. To clarify this fundamental issue, we have studied the mechanism of how the critical points of the first-order valence transitions are controlled by the magnetic field [1]. We show that the critical temperature is suppressed to be the QCP by the magnetic field and unexpectedly the QCP exhibits nonmonotonic field dependence in the ground-state phase diagram, giving rise to emergence of metamagnetism even in the intermediate valence-crossover regime. The driving force of the field-induced QCP is clarified to be a cooperative phenomenon of Zeeman effect and Kondo effect, which creates a distinct energy scale from the Kondo temperature. This mechanism explains a peculiar magnetic response in CeIrIn₅ and metamagnetic transition in YbX₄ₓCdₓ for X=In as well as a sharp contrast between X=Ag and Cd. We present the novel phenomena under the magnetic field to discuss significance of the proximity of the critical points of the first-order valence transition. [1] S. Watanabe et al. PRL100, (2008) 236401.

11:39AM B41.00003 Combined Effects of Magnetic Field and Uniaxial Pressure on CeCoIn₅₁, RENA ZIEVE, SCOOTER JOHNSON, UC Davis, JASON COOLEY, Los Alamos National Laboratory — CeCoIn₅ exhibits unusual behavior in a magnetic field. The upper critical field is highly anisotropic, more than a factor of two larger for a field applied in the ab-plane than for a field along the c-axis. In both field orientations the superconducting transition changes from second-order to first-order with increasing field, and possible FFLO phases have been observed at high fields. Here we explore the influence of uniaxial pressure, applied along the crystal c-axis, on the temperature-field phase diagram. We find that a magnetic field suppresses the superconductivity far more sharply when the sample is also under pressure. We also examine the slope of the phase boundary near zero field and the nature of the transition at higher fields.

1Supported by NSF under DMR-0454869

11:51AM B41.00004 Dependence of Superconducting Transition Temperature on Uniaxial Pressure in CeCoIn₅, SCOOTER JOHNSON, RENA ZIEVE, UC Davis, JASON COOLEY, Los Alamos National Laboratory — We apply uniaxial pressure up to 4 kbar along the c-axis of single crystal samples of CeCoIn₅ and measure how the transition temperature to the superconducting state changes. We mount the sample within an ac susceptibility coil and apply pressure through a helium bellows cell mounted on a dilution refrigerator. We find that pressure shifts the transition to lower temperatures at a rate of 22.5 mK per kbar. Our observation follows the general correlation between transition temperatures and lattice constants among 115 materials, where lower Tc’s typically correspond to smaller c/a ratios. Pressure has the additional effect of broadening the transition well beyond what we expect from macroscopic pressure inhomogeneity. We are extending this work to measurements of CeCoIn₅ under a-b-axis pressure.

1Supported by NSF through DMR-0454869

12:03PM B41.00005 Optical Study of the Heavy Fermion Superconductor CeCoIn₅₁, T. GEBRE, T. TUKUMOTO, J. CHERIAN, T. MURPHY, S. TOSZER, E. PALM, C. WIEBE, S. MCGILL, National High Magnetic Field Laboratory — We have performed dc magnetization and optical spectroscopy on flux-grown crystals of the heavy fermion superconductor, CeCoIn₅. We will discuss the growth technique and report results of low-temperature and high magnetic field measurements for different orientations of field and crystal axis. CeCoIn₅ is a strongly correlated system exhibiting superconductivity below 2.3 K and is believed to show a variety of magnetic field-induced phases near or below the critical temperature.

1This work was sported by DOE-FG52-06NA26193 and NSF DMR-0084173

12:15PM B41.00006 Coexistence of Superconducting and Magnetic Order in CeCoIn₅, GEORGIOS KOUTROULAKIS, VESNA MITROVIC, Brown University, MLADEN HORVATIC, CLAUDE BERTHIER, GHMFL, Grenoble, France, GERARD LAPERTOT, JACQUES FLOQUET, CEA, Grenoble, France — The interplay between magnetic and superconducting order near a quantum critical point in heavy fermion materials has attracted intensive research interest in recent years. One of the most intriguing examples is that of CeCoIn₅, in which a novel phase within the superconducting phase is observed near the critical field at low temperature. Recent nuclear magnetic resonance [1] and neutron scattering [2] experiments showed that a static magnetic order is stabilized in this phase. The microscopic nature of this magnetic state will be discussed.


12:27PM B41.00007 ABSTRACT WITHDRAWN

12:39PM B41.00008 Local Structure and Site Occupancy in Cd- and Hg-doped CeTIn₅ (T=Co, Rh, Ir), C.H. BOOTH, Lawrence Berkeley National Laboratory, E.D. BAUER, F. RONNING, V. SIDOROV, T. PARK, J. THOMPSON, J.L. SARRAO, Los Alamos National Laboratory, A.D. BIANCHI, Z. FISK, UC Irvine — Local structure measurements using the extended x-ray absorption fine-structure (EXAFS) technique were performed on the In K, Cd K, and Hg L₃ edges on samples of CeCo(Inₑ₋ₓCdₓ)₅ (0.5%≤x≤31.3%) and CeT(In₁₋ₓHgₓ)₅ (T=Co, Rh, Ir, 0.7%≤x≤3.5%). Fits indicate no measurable change in the bulk local structure with these substituents. In contrast, the local structure data around the substituent atoms indicates about fₐₐₐ = 44(3)% of Cd atoms reside on In(1) sites, similar to previous results [fₐₐₐ = 35(5)%] for Sn in CeCo(In₁₋ₓSnₓ)₅. Mercury has an even stronger preference for the In(1) site, with fₐₐₐ = 71(5)% and fₐₐₐ = 97(3)%, and fₐₐₐ = 55(5)%, although other phases appear to be present in the Ce(In₁₋ₓHgₓ)₅ material. Small distortions from the parent structure are also observed around the substituent atoms. These results will be related to the sharp decrease in the superconducting transition temperature with x.
12:51PM B41.00009 Cd and Sn doping effects on Pauli limiting and HFLT state in CeCoIn$_5$\textsuperscript{1}. R. MOVSOVICH, Y. TOKIWA, N. KURITA, F. RONNING, E.D. BAUER, P. PAPIN, J.D. THOMPSON, Los Alamos National Laboratory, Los Alamos, NM 87544, USA, A.D. BIANCHI, University of Montreal, Montreal, QC, H3C 3J7 Canada, J.F. RAUSCHER, S.M. KAUZLARICH, Z. FISK, University of California, Davis, California 95616, USA, I. VEKHTER, Louisiana State University, Baton Rouge, Louisiana 70803, USA — We investigated the effect of Cd and Sn doping on the superconducting (SC) transition temperature $T_c$, the superconducting critical field $H_{c2}$, and the High-Field-Low-Temperature (HFLT) phase in heavy fermion superconductor CeCoIn$_5$. $T_c$ decreases monotonically for both dopants, whereas $H_{c2}$ rises initially with Cd substitution, while dropping for Sn doping. Analysis of the magnetization data suggests that these effects are caused by weakening of the Pauli limiting in CeCoIn$_5$ with Cd doping, most likely due to changes of susceptibility of the normal state. Both Cd (leading to AFM ground state at higher concentrations) and Sn impurities, at a very low level of a few hundred ppm, suppress the HFLT phase. We interpret these results as supporting the superconducting origin of the HFLT phase.

\textsuperscript{1}Work at Los Alamos National Laboratory was performed under the auspices of the U.S. Department of Energy.

1:03PM B41.00010 Kondo coherence and superconductivity in Yb doped CeCoIn$_5$. ANDREA BIANCHI, GABRIEL SEYFARTH, BOBBY PREVOST, SJOERD ROORDA, Universite de Montreal, DAN HURT, CIGDEM CAPAN, ZACHARY FISK, Dept. Phys. & Astro. U. of California, Irvine — We have studied the effect of Yb doping on superconductivity in the unconventional heavy fermion superconductor CeCoIn$_5$ in a doping series spanning from pure CeCoIn$_5$ to the paramagnetic metal YbCoIn$_5$, which is isostructural with CeCoIn$_5$. By replacing Ce by Yb, we are at the same time removing carriers as well as disrupting the Kondo lattice of CeCoIn$_5$, which is thought to be responsible for superconductivity in this compound. This will give us insight into how the Kondo coherence and Cooper pair breaking in CeCoIn$_5$ are affected by Yb substitution. Our doping series shows that the unit cell volume stays approximately constant up to a Yb concentration of about 40 %. At higher Yb concentrations the unit cell volume begins to shrink gradually to the value of YbCoIn$_5$. However, superconductivity in the doped system is remarkably resilient against Yb substitution: At low doping the superconducting transition temperature $T_c$ is only gradually suppressed from the value of 2.24 K of pure CeCoIn$_5$, and only with a Yb concentration of 60 % $T_c$ is suppressed below 0.3 K.

1:15PM B41.00011 Conductance asymmetry in point-contact junctions on the heavy-fermion compounds CeMn$_5$ (M=Co, Rh, Ir)\textsuperscript{1}. L.H. GREENE, W.K. PARK, University of Illinois at Urbana-Champaign, E.D. BAUER, J.L. SARRAO, J.D. THOMPSON, Los Alamos National Laboratory — The Ce-based 1-1-5 heavy-fermion compounds CeMn$_5$ (M=Co, Rh, Ir), continue to draw much attention from the community. One of the key questions is how the localized discrete states acquire itinerancy over the conduction electron continuum. As a probe of the evolutionary behavior of the Kondo lattice, we take differential conductance spectra from nanoscale metallic junctions on CeMn$_5$ single crystals over wide temperature ranges. A striking common feature is the systematic development of an asymmetry in the background conductance \cite{1}. Conventional models including the heating model with large Seebbeck coefficients of heavy fermions do not account for this behavior. We propose a phenomenological model based on a possible Fano interference effect \cite{2} between two conductance channels, one into the heavy electron liquid (hybridized f-band) and the other into the conduction electrons without hybridization. \cite{1} W. K. Park et al., Phys. Rev. Lett. 100, 177001 (2008). \cite{2} U. Fano, Phys. Rev. 124, 1866 (1961).

\textsuperscript{1}This work is supported by the U.S. DOE under Award No. DE-FG02-07ER46453 and by NSF-DMR-0706013 through FSMRL and CMM at UIUC and is performed at LANL under the auspices of the U.S. DOE, Office of Science.

1:27PM B41.00012 The Fano effect in the point contact spectroscopy of heavy electron materials\textsuperscript{1}. YI-FENG YANG, Los Alamos National Laboratory — Recent experiments on CeCoIn$_5$ reveal similar temperature dependence of the conductance asymmetry in the point contact spectroscopy and the Knight shift anomaly. This suggests a common origin of both anomalies and supports a previously proposed phenomenological two-fluid model that predicts the emergence of a heavy fluid, or Kondo liquid, in heavy electron materials. Here we propose a phenomenological formula for the point contact spectroscopy and describe the spectra by a Fano effect of tunneling electrons due to the Kondo liquid emergence. Our formula explains quantitatively the experimental data of several heavy electron materials.

\textsuperscript{1}This research was supported by an ICAM Fellowship, UC Davis, and the Department of Energy.

1:39PM B41.00013 Evidence for magnetic field-tuned quantum criticality below $H_{c2}$ in CeCoIn$_5$. J. PAGLIONE, Center for Nanophysics and Advanced Materials, University of Maryland, J.-P. REID, Département de physique, Université de Sherbrooke, M.A. TANATAR, L. TAILLEFER, Département de physique, Université de Sherbrooke, C. PETROVIC, Condensed Matter Physics, Brookhaven National Laboratory — The existence of a magnetic-field-tuned quantum critical point coinciding with the upper critical field for superconductivity in the heavy-fermion superconductor CeCoIn$_5$ has remained a puzzling fact, and has proven difficult to study due to the onset of superconductivity. Here we present low temperature thermal conductivity measurements which probe the quantum critical point in CeCoIn$_5$ as a function of field from within the superconducting state, revealing new evidence for field- tuned quantum criticality.

1:51PM B41.00014 Insulating Vortex Core near QCP in CeCoIn$_5$. H. XIAO, T. HU, C. C. ALMASAN, Department of Physics, Kent State University, Kent, OH, 44242, USA, T. A. SAYLES, M. B. MAPLE, Department of Physics, University of California at San Diego, La Jolla, California, 92093, USA — We have investigated the vortex core of the superclean unconventional heavy fermion superconductor CeCoIn$_5$, by studying the flux flow dissipation in the mixed state for two magnetic field orientations, i.e., $H \parallel c$ axis and $H \parallel ab$ plane, at temperatures down to 1.8 K. The vortex core in the mixed state of CeCoIn$_5$ is insulator-like, in contrast to the metallic behavior of CeCoIn$_5$ in its normal state, at temperatures $T$ larger than the superconducting transition temperature $T_c$. Moreover, the abnormal insulating behavior of the vortex core is strongly suppressed when CeCoIn$_5$ is tuned away from the quantum critical point (QCP) by applying pressure. This latter result gives firm evidence that quantum criticality plays an important role in the interaction between superconductivity and magnetism, hence is responsible for the emergence of unconventional superconductivity. A scaling law of the flux flow resistivity has also been found and will be discussed.

\textsuperscript{1}This research was supported by the National Science Foundation under Grant No. DMR-0705959 at KSU and the US Department of Energy under Grant No. DE-FG02-04ER46105 at UCSD.
The effect of Yb substitution in the heavy-fermion superconductor CeCoIn$_5$\textsuperscript{1}\textsuperscript{,} LEI SHU, E. GONZALES, K. HUANG, T.A. SAYLES, U. Calif. San Diego, California 920931 U.S.A., J. PAGLIONE, U. Maryland, Maryland 20742, U.S.A., M.B. MAPLE, U. Calif. San Diego, California 920931 U.S.A. — The discovery of a new family of heavy-fermion superconductors with the formula CeMn$_5$ (M=Co, Rh, Ir ) provides an interesting playground to understand the relation between unconventional superconductivity and quantum criticality. CeCoIn$_5$, with the highest ambient pressure superconducting transition temperature of all heavy-fermion compounds, exhibits a magnetic field-tuned quantum critical point. The peculiar magnetic properties of CeCoIn$_5$ are determined by the interaction between the magnetic moments of the Ce$^{3+}$ ions and the spins of conduction electrons. Through systematic studies of Ce$_{1-x}$Yb$_x$CoIn$_5$ alloys, where the magnetic Ce ions (4f$^1$ configuration) are diluted by Yb (hole analogue; 4f$^{13}$ configuration), it allows us to study the nature of inter-site interactions. Lattice constant, magnetic susceptibility, and electrical resistivity data of Ce$_{1-x}$Yb$_x$CoIn$_5$ alloys throughout the range 0 ≤ x ≤ 1 will be reported.

\textsuperscript{1}This research was sponsored by the U.S. Department of Energy under Research Grant # DE-FG02-04ER46105 and the National Science Foundation under Grant No. 0802478.

C1.00001 POLYMERIC AND ORGANIC MATERIALS I

C1.00002 High Electric Energy Storage in a Three-Phase Polymer Nanocomposite\textsuperscript{1}, JING WANG, FANGXIAO GUAN, LEI ZHU, Polym. Program, Inst. of Mater. Sci. and Dept. of Chem., Mater. and Biomolecular Eng., University of Connecticut, Storrs, CT 06269-3136 — Two-phase polymer/ferroelectric ceramic composites have attracted great interests for electric applications, such as transducers, piezo-sensors, and hydrophone materials, because they combine good processability of polymers and high dielectric constant of ferroelectric ceramics together. The polymer-ceramic composites generally show a high effective dielectric constant only at a high ceramic volume fraction (>35 vol.%). Here, a high dielectric constant tetrameric Cu-philhalocyanine (Cu-TMPc) was used as an interfacial phase between the ceramic particles (50-nm BaTiO3) and the polymer matrix (poly(vinylidene fluoride-co-hexafluoropropylene), or P(VDF-HFP)). To avoid the agglomeration of nanoparticles in P(VDF-HFP)), poly(methyl methacrylate) is grafted from Cu-TMPc-coated BaTiO3 nanoparticles using surface-initiated radical polymerization. High electric energy storage and low conductivity were achieved at low filling ratios (<15 vol.%).

\textsuperscript{1}This work is supported by Air Force Office of Sponsored Research through Agiltron, Inc.(FA9550-06-C-0074 and FA9550-07-C-0083).

C1.00003 Rheological Singularity near the Phase Transition of Hairy Nanoparticles in Polymer Melts, XIAORONG WANG, Bridgestone Americas, Center for Research and Technology, 1200 Firestone Parkway, Akron, OH 44317, VICTOR FOLTZ, MINDAU GUS RACKAITIS, GEORG BOHM — The dynamics of hairy nanoparticles in polymer melts of chemically identical chains has been investigated as function of both molecular weight and volume fraction. This work demonstrates that there is a strong connection between the rheological dynamics of the system and the thermodynamics of the phase separation behavior. The shear-induced nonlinearity in the system appears to display features of a surprising singularity near the phase transition point. Our theoretical calculation also agrees qualitatively well with that observed experimentally.

C1.00004 The use of the radius of gyration in a WLC polymer model of cancer cell adhesion to glycosaminoglycans substrates, ANTONIO PERAMO, GARRETT MATTHEWS, University of South Florida — Glycosaminoglycans (GAG) are a group of polysaccharides involved in several biological functions, including cell adhesion. Most of their biological properties are derived from the interactions of the chains with their environment, hence the interest in developing physical models that could describe their interactions with whole cells. As linear biopolymers with low polydispersity, GAG can be described using polymer models of Gaussian chain distributions, like the WLC (worm-like chain) model. We found that the adhesion of whole cancer cells to glass substrates coated with GAG appear to be dependent on the charge per dimer and degree of sulfation of the GAG chain. We have hypothesized that the adhesion of whole cancer cells to GAG substrates can be described as a function of polysaccharide radius of gyration and used the WLC model describing the global structure of the GAGs to analyze this relationship. We will show that the adhesion of the cancer cells has a linear response with the radius of gyration and is essentially controlled by the charge per dimer. This dominating mechanism is not eliminated when the cells are resuspended in media with heparin. We then propose how these physical properties could be used to predict the preferred molecular structures of compounds for use as anti-metastatic or anti-inflammatory agents.

C1.00005 Polymer dynamics and ion conduction in modified soluble starch, HYUNGKI LEE, JAMES RUNT, Penn State University — The dynamics of neat and plasticized carboxylated starch is investigated using broadband dielectric relaxation spectroscopy (DRS). The sodium single ion conductor is prepared by a 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO) mediated oxidation process, in which the primary hydroxyl groups in alpha-D-glucose units are replaced by carboxylic salts. DRS measurements show that the ionic conductivity increases with increasing degree of oxidation. For example, 78 percent carboxylated starch with 25 weight percent glycerol displays around 3 orders of magnitude higher ionic conductivity than the comparable glycerol-plasticized 25 percent carboxylated material, principally due to the higher content of mobile cations. The role of salts and plasticizers including water on the relaxation behavior of amylose-rich starch is explored. Other complimentary techniques are used in the investigation, including FTIR, XRD and DSC.

\textsuperscript{1}Supported by the USDA CSREES program

C1.00006 Responsive Block Copolymer and Gold Nanoparticle Hybrid Nanotubes, SEHOON CHANG, SRIKANTH SINGAMANENI, SETH YOUNG, VLADIMIR TSUKRUK, Georgia Institute of Technology — We demonstrate the facile fabrication of responsive polymer and metal nanoparticle composite nanotube structures. The nanotubes are comprised of responsive block copolymer, polystyrene-block-poly(2-vinylpyridine) (PS-b-P2VP), and gold nanoparticles. PS-b-P2VP nanotubes were fabricated using porous alumina template and in situ reduction of the gold nanoparticles in P2VP domains. Owing to the pH sensitive nature of P2VP (anionic polymer with a pK$_a$ of 3.8), the nanotubes exhibit a dramatic change in topology in response to the changes in the external pH. Furthermore, the gold nanoparticles in the responsive block exhibit a reversible aggregation, causing a reversible change in optical properties such as absorption.
C1.00007 Magnetic Field Alignment of Rod-Coil Block Copolymers and Identification of Liquid Crystalline Orientation, X. GU, University of California, Berkeley, B.D. OLSEN, A. HEXEMER, E. GANN, R.A. SEGALMAN, UC BERKELEY TEAM, LAWRENCE BERKELEY LABS TEAM — Conjugated rod-coil block copolymers are potentially useful for a number of optoelectronics applications, but properties rely strongly on the orientation of both the conjugated rods and of the nanodomains. Here, a magnetic field was used to control the self-assembly of a model conjugated rod-coil block copolymer (poly(alkoxyphenylenevinylene-b-isoprene)) such that the rods align with the field direction. After alignment, the samples were re-annealed below the microphase order-disorder transition temperature to allow equilibration of the rod orientation within the lamellar nanodomains. Small angle and wide angle X-ray scattering simultaneously determine the rod tilt relative to the lamellar normal. Rods were found to be parallel to the lamellar plane by fractions of 42-85 percent at all temperatures below the microphase order-disorder transition temperature. The orientation of the rod blocks in rod-coil block copolymers impacts carrier transport and optical properties in organic electronic devices, making the control of rod orientation necessary for device optimization.

C1.00008 A New Level of Hierarchical Structure Control by Use of Supramolecularly Assembled Dendronized Block Copolymers, RAFFAELE MEZZENGA, CHAOXU LI, University of Fribourg, Switzerland, DIETER SCHLUTER, AFANG ZHANG, ETHZ, Switzerland — Block copolymers in which microphase segregation can be combined with supramolecular attachment of side chains to one block, constitute very appealing systems to design hierarchically self-assembled macromolecular materials. Self-organization of these systems is achieved at two length scales: that of the side chains (~10^1 nm) and that of the block copolymers (~10^-10^7 nm). Because of the linear nature of the hosting block, only lamellar organization is typically observed at small length scales. Here we demonstrate that by replacing the linear polymer block with a dendronized polymer capable of participating in supramolecular interactions, one additional degree of freedom (the generation of the dendronized polymer) is introduced to engineer the self-assembly into unprecedented hierarchically ordered bulk structures. Not only this allows controlling beyond current possibilities the structures at the smaller length scale, with the introduction for example, of new columnar rectangular, hexagonal and tetragonal phases, but it may also lead to new functional template materials with increased 3D topological complexity for advanced technologies. References: C. Li, D.A. Schlüter, A. Zhang, R. Mezzenga, Advanced Materials, in press.

C1.00009 Fabrication of Highly Ordered Nanostructured Block Copolymer Templates using Supramolecular Assembly Approach, E. BHOJE GOWD, MANFRED STAMM, LEIBNIZ INSTITUTE OF POLYMER RESEARCH DRESDEN, HOHE STRASSE 6, 01069 DRESDEN, GERMANY TEAM — The ability to create reactive nanoporous templates using polymer thin films is important for such applications as antibody or enzyme immobilization, separation of biomolecules, and nanofabrication. Self-assembly of polymers supramolecularly with C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-b-dimethylsiloxane) thin films disordered leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60-fullerenes to poly(styrene-dimethylsiloxane) thin films leads to disorder in a system that is otherwise ordered in the range of tens of microns.

C1.00010 Neutron Reflectivity Study of dPS Brushes Grown from an Inimer Embedded Polymer Matrix, ONOME SWADER, Department of Chemistry, University of Tennessee, Knoxville, TN, DAMLA KOYLU, KENNETH CARTER, Polymer Science and Engineering Department, University of Massachusetts, Amherst, MA, MARK DADMUN, Department of Chemistry, University of Tennessee, Knoxville, TN — Robust methods for directing the self-assembly of macromolecules over large areas are necessary in order to meet the demands for fabrication of next generation devices. Polymer brushes grown from soft interfaces composed of an inimer embedded photopolymer (PP) network provide a unique method to create tuned surfaces and interfaces for such devices. In this study, neutron reflectivity is used to characterize such functionalized interfaces. Intermolecular concentration and the amount of monomer available for polymerization was systematically varied in an attempt to nanoscopically tune brush growth. These results suggest that the brushes are not initiated at one particular interface, but rather throughout the PP network. Further analysis revealed that brush density increased as the amount of inimer concentration in the PP network increased. However, it is interesting to note that the brush at the surface of the PP network is significantly less dense than in the melt.

C1.00011 Surface Dynamics of Branched Polystyrene films, SHIH-FAN WANG, JAE SIK LEE, SEWOO YANG, RODERIC P. QUIRK, MARK D. FOSTER, Dept. of Polymer Science, University of Akron, ZHANG JIANG, SURESH NARAYANAN, X-ray Science Division, Argonne National Lab, DAVID WIU, Colorado School of Mines — Thermally stimulated fluctuations of a polymer surface have been studied for films containing branched polymers for the first time. The surface fluctuations were recorded using X-ray photon correlation spectroscopy (XPCS), a recently-developed technique already applied to study the surfaces of melts of linear polystyrene chains. A continuum hydrodynamic theory of thermally stimulated capillary waves with a non-slip boundary condition is adequate to fit plots of relaxation time as a function of scattering vector. Changes in Tg with molecular architecture certainly play a role. However, comparison of data from a star made without the usual butadiene (BD) linking units with data from a star with 1-2 BD units per arm shows that the BD end capping of the arms affects the dynamics profoundly. This effect may not be described adequately by simply accounting for the reduction in Tg caused by the presence of the BD units. Acknowledgements: NSF support (CBET 0730692)

C1.00012 Magnetic Field Driven Alignment of Lamellar and Hexagonal Surfactant Mesophases for Templated Synthesis of Nanomaterials, PAWEI MAJEWSKI, CHINEDUM OSUJI, Yale University — The use of both ionic and non-ionic surfactants as structure directing agents in the solvothermal synthesis of nanomaterials has become a well established practice. Nevertheless, the production of monolithic well aligned surfactant mesophases for use in the templated synthesis of ordered, anisotropic nanomaterials remains a significant challenge, particularly in the thin film geometry where shear alignment cannot be conveniently applied. Magnetic fields hold promise in this area, but to date have only been used in the alignment of hexagonal phases of ionic surfactants. We show that judicious application of high magnetic fields can in fact be used for diamagnetic alignment of non-ionic surfactants in both the lamellar and hexagonal phases, leading to very highly ordered systems suitable for nanomaterials synthesis.

C1.00013 Long Range Order of Block Copolymer/C60 Thin Films, KATIE CAMPBELL, DAVID BUCKNALL, YONATHAN THIO, Georgia Institute of Technology — The use of block copolymers as a template to localize C60 particles was investigated. The addition of C60-fullerenes to poly(styrene-b-dimethylsiloxane) thin films led to disorder in a system that is otherwise ordered in the range of tens of microns. Because C60 segregates into the PS phase, the degree of disorder is dependent on the concentration of C60 as a weight percent of the PS block, as indicated by AFM studies. Disorder effects are exacerbated by fullerene aggregation in the solution prior to spin coating on a substrate. Several strategies are proposed for achieving and maintaining long-range order in block copolymer/C60 thin films. First, the aggregation of C60 in solution is controlled by preparing thin films from solutions with C60 and block copolymer co-dissolved at a time when aggregation is at a minimum to achieve good dispersion of the C60. Secondly, several methods for achieving long-range order have been investigated including the use of solvent annealing in combination with shear and topographic substrates. Results show that solvent annealing alone orients polymer segments in C60-fullerene copolymers without C60; however, addition of C60 to the system alters the order seen with solvent annealing.
C1.00014 Orientation distribution in a uniaxially and biaxially drawn poly(L-lactic acid) by Raman spectra, MIN SANG PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, Atlanta, GA, USA, YEE SHAN WONG, SUBBU VENKATARAMAN, School of Materials Science and Engineering, Nanyang technological University, Singapore, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA — In this study, we used the polarization modulation of Raman scattering intensities to study molecular orientation distribution in the crystalline and amorphous regions of uniaxially and biaxially drawn poly(L-lactic acid) (PLLA) film. Changes of orientation distribution were detected as a function of stretching ratios and different characteristics of orientation between crystalline and amorphous region were analyzed using Raman bands which are assigned to the each region. As results, quantification of oriented molecule information named orientation order parameters was determined. From experimentally obtained order parameters, the most probable molecular orientation distribution functions for the crystalline and amorphous regions in the film could be constructed.

C1.00015 Highly Ordered Nanoporous Template from ABC Triblock Copolymer, DONG HYUN LEE, SOOJIN PARK, THOMAS RUSSELL, Univ of Massachusetts, Amherst — In this study, silicon nanoporous templates from polyisopropene-block-polystyrene-block-poly(2-vinyl pyridine) (PI-b-PS-b-P2VP) were fabricated. The films, spin-coated from toluene, showed a dimpled texture with short-range lateral order. When exposed to a mixed solvent vapor (toluene/hexane), a highly ordered and oriented core-shell structure of PI-b-PS-b-P2VP copolymers was obtained. The morphology consisted of an external shell of PI, a middle shell of PS, and a core of P2VP. After removal of the PI from by UV-Ozone treatment, subsequently, polydimethylsiloxane (PDMS) was spin coated onto this film and allowed diffused into the pores by capillary action. When the film was exposed to oxygen plasma, the PDMS was converted to silicon oxide, while all other remaining polymer was removed. This led to a highly ordered and oriented nanoporous structure that could be used as an etching mask or templates for secondary metal loading. Highly ordered arrays of gold nanoparticles for the potential applications for surface enhanced plasmon, immobilization of DNA or organic dyes, or epitaxial growth of crystal were obtained by loading gold salt into well-defined core-shell structure.

C1.00016 Morphology and Ionic Conductivity of Block Copolymer–Ionic Liquid Systems, M.L. HOARFROST, J.M. VIRGIL, J.B. KERR, R.A. SEGALMAN, UC Berkeley and Lawrence Berkeley National Laboratory — Block copolymer–ionic liquid systems are of interest for ion exchange membranes due to the ionic conductivity and thermal stability of the ionic liquid combined with the thermal stability and morphological control arising from a structural component in a block copolymer. It is anticipated that the morphology and connectivity of the resulting structural and ionic liquid-containing nanodomains will affect conduction properties. This relationship was investigated for poly(styrene-b-2-vinylpyridine) (S2VP) in ionic liquids composed of varying molar ratios of imidazole and bis(trifluoromethanesulfonfyl)imide (Im:TFSI). A stoichiometrically balanced ionic liquid (1:1 Im:TFSI) swells the 2VP lamellar domains for copolymer concentrations as low as 60wt%. With 9:1 Im:TFSI the lamellar structure tolerates more swelling, forming lamellar structures with as little as 30wt% copolymer. Ionic conductivity in two-dimensional and three-dimensional systems, characterized by microphase separated domains, demonstrate ionic conductivities comparable to those of P2VP–ionic liquid systems when normalized by 2VP (monomer) to Im:TFSI ratio.

C1.00017 Ionic Salt Effect on the Phase Transition of PS-b-P2VP Copolymers, BOKYUNG KIM, HYUNGJU AN, DU YEOL RYU, Yonsei University, Korea, JEHAN KIM, Pohang Accelerator Laboratory, Korea — Solid-state electrolytes have long been considered as suitable candidates owing to the simple and easy processes for rechargeable battery manufacture, compared to conventional liquid electrolyte counterparts. Especially, polymer/salt systems involving PMMA and PVP complex forms have been studied since they provide stable electrochemical characteristics as well as mechanical properties. We studied the phase behavior of PS-b-P2VP upon the salt addition by small angle x-ray scattering (SAXS) and depolarized light scattering. Transition temperatures of block copolymer were significantly influenced by the salt addition in addition to the changes of d-spacings, which is caused by the effective coordinative interaction between P2VP block and salt. This study suggests a simple approach to solid-state block copolymer electrolytes.

C1.00018 Comb Polymer Architectures for Versatile Nanoparticle Assembly, ALEXANDER MAS-TROIANNI, KARI THORKELSSON, YUE ZHAO, JOSEPH LUTHER, JILL MILLSTONE, PAUL ALIVISATOS, JEAN FRECHET, TING XU, UC Berkeley — Nanoparticles are a material of interest in photovoltaic research due to their optical absorption properties. However, there have been many challenges for device fabrication. Nanoparticle-doped organic thin films are a hot area of research, and they have thus been hard to apply generally to different materials of interest. We show how this challenge can be overcome using a comb polymer architecture. Here, pentacetyphenol small molecules are hydrogen bonded to polyvinyl pyridine. This alkyl moiety is compatible with the ligand shells of many nanomaterials. We incorporated these small molecules and nanoparticles into polystyrene-polyvinyl pyridine block copolymers. This strategy was successful for assembling nanoparticles, made out of a variety of materials, without special considerations for the actual core material or morphology. Following these successes in bulk samples we extended our studies to thin films of these composites. Here, the morphology is controlled by the interfacial interactions. These materials have the potential to be used for photovoltaic devices, as they are easily solution-processable. This strategy is generally applicable with the choice of small molecule mediating interactions with any desired nanomaterial.

C1.00019 Electric Energy Storage in P(VDF-HFP) Copolymers with Different Crystallinities, FANGXIAO GUAN, STEVEN BOOGS, LEI ZHU, Polym. Program, Inst. of Mater. Sci. and Dept. of Chem., Mater. and Biomolecular Eng., University of Connecticut, Storrs, CT 06269-3136 — Poly(vinylidene fluoride) (PVD) is a well known ferroelectric polymer. It attracts much attention as a candidate material for electric energy storage in recent years because of its relatively high dielectric constant and high electric breakdown strength. By modifying PVDF with bulky comonomers such as hexafluoropropylene (HFP), (P(VDF-HFP) random copolymers can achieve even higher electric energy density than PVDF. This is because bulky HFP comonomers disrupt the PVDF run length and thus reduce the average crystallite size. Additionally, bulky HFP comonomers at the crystal surface constrain the α- → δ- → β phase transitions at elevated electric fields. Both the reduced crystallite size and constrained phase transition affect electric energy storage. For (P(VDF-HFP) copolymers with different crystallinities, different crystal size and phase transition behaviors are studied, and their relationships with the electric energy storage capability is correlated.

C1.00020 Multi-scale simulation on solid benzene, HUA LIU, HENDRIK HEINZ — Solid Benzene is used in organic semiconductors for photovoltaics, which often include pi-conjugated systems. We use MD simulations method to explore the relationship between the structure and interaction energy of two kinds of solid benzene, with the Pbcn and P21c crystallographic structures respectively. Simple relevant force fields (PCFF and CVFF) are examined with regard to their performance on the structure and energetics of benzene dimers and benzene crystals which serve as well characterized model systems. However, MD simulations cannot get the transport properties. So the combination of reliable classical atomistic simulations and quantum-mechanical methods is needed to understand the dynamics of charge transport and self-assembly processes involving pi-conjugated oligomers and polymers. As alternative and accurate models, we explore atomistic models with additional sites which represent the location of the pi electrons and are characterized by suitable charges and van-der-Waals parameters. With these parameters, it will be possible to reproduce the dimer geometries and energies, the crystal structure of solid benzene, as well as pi-stacking forces and free energies for similar systems.
The surface spectrum of PS films subjected to different thermal annealing, we show that similar nonliquidlike behaviors can be produced if the annealing time is below \( \tau(q_{eq}(h)) \), the relaxation time of the capillary wave mode with wave vector equal to the lower-cutoff wave vector \( q_{eq}(h) \), which characterizes the equilibrium surface spectrum. At the same time, annealing above \( \tau(q_{eq}(h)) \) recovers the liquid behaviors. Because \( \tau(q_{eq}(h)) \) often amounts to days and even years, insufficient annealing constitutes a likely cause for the nonliquidlike behaviors. Nonetheless, the previously suggested strong pinning of the polymer chains to the substrate can also be a cause. To elucidate the origin of the observed nonliquidlike behaviors, we measure the surface dynamics of PS films with thicknesses of \( h \approx 2R_C \) (where \( R_C \) is the radius of gyration of the polymer) exhibited nonliquidlike behaviors even in the molten state. By measuring the surface spectrum of PS films subjected to different thermal annealing, we show that similar nonliquidlike behaviors can be produced if the annealing time is below \( \tau(q_{eq}(h)) \), the relaxation time of the capillary wave mode with wave vector equal to the lower-cutoff wave vector \( q_{eq}(h) \), which characterizes the equilibrium surface spectrum. At the same time, annealing above \( \tau(q_{eq}(h)) \) recovers the liquid behaviors. Because \( \tau(q_{eq}(h)) \) often amounts to days and even years, insufficient annealing constitutes a likely cause for the nonliquidlike behaviors. Nonetheless, the previously suggested strong pinning of the polymer chains to the substrate can also be a cause. To elucidate the origin of the observed nonliquidlike behaviors, we measure the surface dynamics of PS films with thicknesses of \( h \approx 2R_C \) to \( 8R_C \) undergoing the glass-to-rubber transition and find that they are all the same. Our result favors insufficient annealing to be the cause of the observed nonliquidlike behaviors.

We thank support of NSF (DMR0706096) and ACS PRF (47882AC5). L. T. thanks support of the Boston University UROP program.

Preparation of Mesoporous Ceramics from Polymer Nanotubes, DIAN CHEN, SOOJIN PARK, JIUN-TAI CHEN, EMILY REDSTON, THOMAS RUSSELL, University of Massachusetts Amherst — Poly(styrene-b-4-vinylpyridine) (PS-b-P4VP) nanotubes were prepared by placing polymer solution into the cylindrical nanopores of an anodic aluminum oxide (AAO) membrane. The PS-b-P4VP nanotubes within the AAO membranes were exposed to tetrahydrofuran vapor to produce uniform spherical micelles along the tube. The tubes were removed from the membranes, then suspended in ethylene glycol, a preferential solvent for P4VP. At 95°C, near the glass transition temperature (Tg) of PS, nanotubes with uniform nanopores were obtained by a reconstruction of the nanotubes. As the temperature was increased, mesoporous polymer structures were obtained. Tetraethyl orthosilicate or titanium tetraoxide, ceramic precursors, were introduced into the 4VP microdomains. After exposure to an oxygen plasma or high temperature, the copolymer was removed and the precursor converted to a mesoporous ceramic. This process offers a simple route for the fabrication of tunable mesoporous ceramic or metallic structures by changing molecular weight of copolymers.

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C1.00028 A Generic Fourier-Space Approach for Discovering Ordered Phases of ABC Star Triblock Copolymers

C1.00029 Collapse Transitions in Thermosensitive Alternating Copolymers: A Monte Carlo Study

C1.00030 Dynamics of Polystyren (PS) Melts: Multi-Scale Molecular Dynamic (MD) Approach

C1.00031 Differential AC-chip nanocalorimeter for measurements at low pressure

C1.00032 Phase Stability in Nanoparticle/Homopolymer Thin Film Mixtures

C1.00033 Healing of Crack on Brittle Substrate by Dual Cross-Linked Nanogel Coating

C1.00034 Design of responsive polymer surfaces with ultrafast response time
C1.00035 Swelling Behavior of Diblock Copolymer Brushes. BULENT AKGUN, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, SUSHIL SATIJA, Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, GOKCE UGUR, MARK D. FOSTER, Department of Polymer Science, The University of Akron, Akron, OH 44325 — Diblock copolymer brushes (DCBs) have garnered enormous interest in recent years due to their stimuli-responsive behavior. The characteristics of a surface of a DCB can be changed reversibly from those of one type to those of another by using a selective solvent for one block. There has not been any experimental study to prove either the disordered structure or the surface rearranged structure or the mechanism of that rearrangement. To understand the switching mechanism we have investigated the swelling behavior of DCBs in selective and good solvents using in-situ neutron reflectivity. When DCBs are treated with selective solvents, in-situ measurements show that the structure changes to minimize the unfavorable interaction between solvent and the block that does not like the solvent. When swollen with a liquid solvent good for both blocks, DCBs behave similarly to homopolymer brushes, establishing a parabolic profile of chain segment density.

C1.00036 Effect of density and structure on dynamics within self-assembled monolayers. DERRICK STEVENS, MARY SCOTT, JASON BOCHINSKI, LAURA CLARKE, NC State University Dept. of Physics — Previously, we have observed interacting dynamics within self-assembled alkylsiloxane monolayers, and characterized this motion via sensitive dielectric spectroscopy (along with more traditional techniques such as ellipsometry, contact angle, and force microscopy). In these monolayers, molecules are covalently bound to the surface and thus cannot spontaneously change density, as in an adsorbate system. We identified this relaxation as akin to the polyethylene-like glass transition observed in polymers with phase-segregated alkyl side chains [1]. As a next step, we deliberately manipulated the physical structure of the monolayers (via different film growth procedures and/or post-deposition heat treating) and the monolayer density (from ~10% to full coverage), and observed the resultant changes in dynamics. This experimental system may prove a useful model for more complex materials, such as glassy polymers or traditional molecular glasses, where density cannot be explicitly tuned. As density increases, the steepness index increases, indicating a more complex or fragile relaxation. At low densities, the motion has an almost-Arrhenius dependence on temperature. [1] M.C. Scott, D.R. Stevens, J.R. Bochinski, L.I. Clarke, ACS Nano. DOI: 10.1021/nn800543j.

C1.00037 Partial Crystallinity in Alkyl Side Chain Polymers. VASAV SAHNI, SHISHIR PRASAD, JOHANNA VILLATE, ZHANG JIANG, SUNIL SINHA, ALI DHINOJWALA, THE UNIVERSITY OF AGRON COLLABORATION, UNIVERSITY OF CALIFORNIA, SAN DIEGO COLLABORATION — Surface freezing is the formation of a crystalline monolayer at the free surface of a melt at a temperature \( T_s \), a few degrees above the bulk freezing temperature, \( T_b \). This effect, i.e. \( T_s > T_b \), common to many chain molecules, is in marked contrast with the surface melting effect, i.e. \( T_s < T_b \), observed for all other materials in the same state. Similarly, \( T_s \) is also > \( T_b \) for temperatures below \( T_b \) at which the surface freezes before the bulk. We have studied the structure of a novel crystalline surface monolayer on top of a disordered melt of the same material (poly(n-alkyl acrylate)) using grazing incidence x-ray diffraction. The grazing incidence x-ray diffraction, surface tension, and bulk latent heat results show that there is partial side-chain crystallinity. Also, the surface tension results explain the trend of the difference between the surface order-to-disorder transition temperature and the bulk melting temperature (\( \Delta T \)) as a function of side chain length. The behavior of the crystal length, crystal spacing and tilt with varying alkyl chain length and temperature was also studied.

C1.00038 Modifying material surfaces by siloxane-based coatings. ALI OZCAM, JAN GENZER, NC State University — We report on a simple, robust, and rapid method of modifying materials surfaces by using poly(vinylmethyl siloxane)-trichlorosilane (PVMS-TCS) coating. PVMS-TCS is synthesized by hydrosilation coupling between trichlorosilane (TCS) and poly(vinylmethyl siloxane) (PVMS). Spin-coating PVMS-TCS onto a substrate results in a uniform coating layer, which can be further stabilized by cross-linking. Exposing the coating to minute amounts of moisture generates a large density of surface-bound hydroxyl groups on the surface of PVMS-TCS. Moreover, by treating the PVMS-TCS substrates with ultraviolet/ozone (UVO) treatment increases one can both further increase the density of the surface-bound hydroxyl groups and the coating’s elastic modulus. The applicability of PVMS-TCS and PVMS-TCS/UVO coatings was tested by decorating various surfaces, including, poly(ethylene terephthalate) and glass, with semifluorinated organosilanes and organosilane-based initiators for surface initiated polymerization. The physico-chemical properties of the functional coatings were studied with a battery of experimental probes, including near-edge x-ray absorption fine structure spectroscopy, x-ray photoelectron spectroscopy, contact angle, atomic force microscopy, ellipsometry, and nanoindentation.

C1.00039 Carbon Nanotube Intra-connects With Conductive Polymers. SEON WOO LEE, HAIM GREBEL, Electronic Imaging Center at NJIT and the Electrical and Computer Engineering Department, New Jersey Institute of Technology (NJIT), Newark, NJ 07102, ANDREI SIRENKO, Physics Department, New Jersey Institute of Technology (NJIT), Newark, NJ 07102, DANIEL LOPEZ, AVI KORNBLIT, New Jersey Nanotechnology Consortium (NJNC), Lucent Technologies Bell Labs, Murray Hill, NJ 07974 — The electrical and optical properties of carbon nanotube (CNT) channels, electroplated with conductive polymers were measured. Individual, single-walled CNT (SWCNT) channels were grown by chemical vapor deposition (CVD) technique between very sharp metal tips on a wafer. The conductive polymers, either polycarbazole (PCz) or, polypyrrole (PPy) were then electroplated using the CNT as an electrode. Field effect transistors were fabricated and a gate-controlled, N-shaped negative differential resistance (NDR) was observed. A large photoconductance effect, which was associated with the NDR, was demonstrated, as well.

C1.00040 Orientation Dynamics in Multi-Wall Carbon Nanotube Dispersions under Shear Flow. SASWATI PUJARI, Northwestern University, SAMEER RAHATEKAR, JEFFREY GILLMAN, National Institute of Standards and Technology, KRZYSZTOF KOZIOL, ALAN WINDLE, Cambridge University, WESLEY BURGHARDT, Northwestern University. We report studies of the orientation state of multi-wall carbon nanotubes (MWNTs) dispersions in steady and transient shear flows. Uncured epoxy was used as a viscous, Newtonian suspending medium, and samples were prepared from ‘aligned’ MWNTs. Orientation was studied in both the flow- gradient (1-2) and flow-vorticity (1-3) plane of simple shear flow using in-situ x-ray scattering techniques. Steady state measurements in the 1-2 plane indicate that the MWNT orientation is rate dependent, with the MWNTs orienting closer to the flow direction at higher shear rates. In steady shear, anisotropy was measured to be higher in the 1-2 plane than in the 1-3 plane, demonstrating that the nanotube orientation state is not uniaxially symmetric in shear. The steady state MWNT orientation is governed by a rate-dependent state of nanotube aggregation/dissociation, which was separately characterized by optical microscopy. A partial relaxation of flow-induced anisotropy was observed following flow cessation, despite the very small rotational diffusivity estimated for these nanotubes. Long transients are observed in step-down experiments, as the orientation state changes in response to the slow tube aggregation process.

C1.00041 Defect Structures in Block Copolymer/Nanoparticle Blends. HYUN JU RU, MICHAEL BOCK-STALLER, Carnegie Mellon University — We present a systematic study of the implications of nanoparticle additives on the defect formation in block copolymer/nanoparticle blends (BCP). The morphology of lamellar styrene/isoprene-based di- and triblock copolymers blended with polystyrene-coated gold nanocrystals at various filling fractions have been done to characterize the monolayer formed when using electron microscopy using stereology and image reconstruction. Three structural characterizations, i.e. the grain size distribution, grain orientation distribution and grain boundary distribution, were analyzed as a function of polymer chain architecture, particle filling fraction and film processing conditions. With increasing particle filling fraction the average anisotropy as well as average grain size is observed to decrease as is the rate of grain growth during thermal annealing. The results are interpreted in terms of the stabilization of grain boundary structures through segregation of particle fillers to the grain boundary regions.
C1.00042 Effect of Nanoparticle Core Size on Polymer-Coated Gold Nanoparticle Location in Block Copolymers . J. D. PETRIE, G. H. FREDRICKSON, E. J. KRAMER, UCSB — Gold nanoparticles modified by short chain polymer thioles [Au-PS] can be designed to strongly localize either in the PS domains of a polystyrene-b-poly(2-vinylpyridine) [PS-PVP] block copolymer or at the interface. The P2VP block has a stronger attractive interaction with bare gold than the PS block. Thus, when the areal chain density \( \Sigma \) of end-attached PS chains falls below a critical areal chain density \( \Sigma_c \), the Au-PS nanoparticles adsorb to the PS-b-P2VP interface. The effect of the polymer ligand molecular weight on the \( \Sigma_c \) has been shown to scale as \( \Sigma_c \sim ((R - R_g)/(R^*R_g))^2 \), where \( R \) is the curvature of the Au nanoparticle core radius. To test this scaling relation for \( \Sigma_c \) further we are synthesizing gold nanoparticles with different core radii and will present preliminary results on \( \Sigma_c \) as a function of \( R \).

C1.00043 Segmental dynamics in poly(cyclohexyl methacrylate) / poly(alpha-methylstyrene) blends . GARETH ROYSTON, PAUL SOTTA, DIDIER LONG, Laboratoire Polymères et Matériaux Avancés (FRE2911) — Study of the dynamics of polymer blends near the glass transition and remains of great current interest. We present broadband dielectric spectroscopy and mechanical spectroscopy data from miscible blends of poly(cyclohexyl methacrylate) and poly(alpha-methylstyrene) across the entire composition range. Results are compared to known data on a range of other systems.

C1.00044 Surface segregation of end-functionalized homopolymers in a homopolymer matrix . MICHAEL DIMITRIOU, UCSB, CHENG WANG, KRISTIN SCHMIDT, HARALD ADE, CRAIG HAWKER, EDWARD KRAMER — Surface segregation of end-functional poly(2-vinylpyridine) in a blend with P2VP was measured by X-ray photoelectron spectroscopy. A series of chain end functionalized P2VP homopolymers were synthesized via either anionic polymerization or Reversible Addition Fragmentation Chain Transfer (RAFT) and end capped with either a single fluorinated oligomer or a perfluorinated dendrimer. The degree of end functionalization was characterized using NMR spectroscopy, IR spectroscopy and gel permeation chromatography. Further surface characteristics were determined using Near Edge X-ray Absorption Fine Structure Spectroscopy and Resonant Soft X-ray Reflectivity. When Swt\% P2VP end capped with a perfluorinated dendrimer was added a top layer saturated with fluorocarbons formed. It was also found that the surfactant segregation is dependant on its ability to form micelles.

C1.00045 Co-crystallization of Alkanes with Longer Methylene Segments within a Statistically Random Copolymer . JEFFREY KALISH, University of Massachusetts-Amherst, SURIYAKALA RAMALINGHAM, YUNING YANG, SHAW LING HSU, University of Massachusetts-Amherst, HENKE COLLABORATION — Binary blends of alkanes \( (C_hH_{2n+2}, n=24, 32, 36) \) and statistically random ethylene-co-vinyl acetate (EVA) copolymers with different vinyl acetate (18, 28 and 40\%) contents have been studied to understand the phenomenon of co-crystallization of longer chain fractions. Using thermal fractionation, the distribution of various crystallizable ethylene chain sequences was established in EVA copolymers. Co-crystallization in blends was observed by changes in spectroscopic features of various unit cells (triclinic, even n=26; monoclinic, even n=26 and orthorhombic, odd n) using vibrational spectroscopy. In order to distinguish these changes, deuterated alkanes were blended with EVA. Orthorhombic unit cells show a doublet in the C-H rocking region due to crystal field splitting; this splitting was removed upon co-crystallization. In Raman spectra, the Longitudinal Acoustic Modes (LAM) are used to validate co-crystallization. LAM did not change significantly when an alkane was co-crystallized with EVA in comparison to the neat alkane. The Raman C-H stretching region changed when a monodispersed alkane was blended. Thermal and X-ray analysis support these spectroscopic results upon co-crystallization.

C1.00046 Phase Behavior of a Weakly Interacting Polystyrene and Poly(n-hexyl methacrylate) System . HYUNGJU AHN, SUDHAKAR NAIDU, DU YEOL RUY, Yongsei University, Korea, JUNHAN CHO, Dankook University, Korea — Understanding the phase behavior of multipolymer material systems has been of great concern to polymer science community, since this provides us a key to the compatibility in most applications involving polymer blends and block copolymers. In the weakly interacting binary blends, UCST-type polymer blends generally undergo a transition from the homogeneous to phase-separated state at the unfavorable segmental interactions, while LCST-type blends show an opposite tendency as a consequence of thermal compressibility (or thermal expansion) difference between two components. We report an experimental evidence for the coexistence of both UCST and LCST behavior in a weakly interacting deuterated PS (dPS) and PnHMA blend system. A new phase diagram involving both UCST and LCST was obtained by the delicate control of molecular weights between dPS and PnHMA. Whereas for the block copolymers such as deuterated polystyrene-b-poly(n-hexyl methacrylate) (dPS-b-PnHMA) and PS-b-PnHMA, an order-to-disorder transition (ODT) on heating was observed within experimental temperature range depending on the molecular weight.

C1.00047 Polydisperse Block Copolymer Melts: Beyond the Schulz-Zimm Distribution . NATHANIEL LYND, Department of Chemical Engineering and the Materials Research Laboratory, University of California, Santa Barbara, MARC HILLMYER, Department of Chemistry, University of Minnesota, MARK MATSEN, Department of Mathematics, University of Reading — Using self-consistent mean field theory, we compared the effects of polydispersity on the phase behavior of block copolymer melts possessing two distinct distributions: the Schulz-Zimm distribution (SZD), and a realistic distribution resulting from a numerical simulation of the kinetics of an equilibrium polymerization (EQD). When the polydispersity indices (PDIs) were matched, the SZD and EQD imparts significant differences in the number of chains pulling free of the interface. This resulted in large differences in domain spacing, but negligible differences in phase boundaries.

C1.00048 Network Phase Behavior of ABC Triblock Copolymer-Homopolymer Blends for Nanoporous Membranes . MAEVA TUREAU, THOMAS H. EPPS, III, University of Delaware — ABC-type block copolymers exhibit morphological diversity not found in diblock copolymers and are becoming a versatile route to nanoscale devices. ABC triblocks are capable of self-assembling into triply-periodic network structures with a high degree of internal interfacial area and tailored chemical and mechanical properties. These unique characteristics make ABC triblock network structures ideal candidates for nanoporous membranes. Our work focuses on the morphological behavior near the network phase window in the poly(isoprene-b-styrene-b-methyl methacrylate) (ISM) system using neat triblocks and selective homopolymer blending. Morphological characterization is accomplished through a combination of small angle X-ray scattering (SAXS), transmission electron microscopy (TEM), and dynamic mechanical analysis (DMA) techniques. Neat triblocks exhibit network structures while blended systems show phase transitions including an alternating gyroid to lamellar phase transition. The neat and blended systems are mapped on a phase diagram to locate the network phase window.

C1.00049 Solution self-assembly behavior of block copolymer blends with restricted hydrophilic block . JIAHUA ZHU, SHENG ZHONG, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware, KENNETH HENRY DEWIS, DARRIN POCHAN, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware — Novel assembled structures due to segregation of hydrophobic domains trapped within the same micelle core have been produced via a block copolymer blend in tetrahydrofuran/water solution. The block copolymer blend is composed of two or more block copolymers with shared polycrylic acid (PAA) hydrophilic block, but distinctive hydrophobic blocks. The blended micelles are created by taking advantage of the electrostatic association in the hydrophilic PAA shell between the negatively charged acid of the PAA block and added, positively charged organamine molecules. Unlike hydrophobic blocks undergo local segregation. This segregation gives rise to new nanostructures deviated from traditional polymeric assemblies such as spheres, cylinders and vesicles. Transmission electron, cryogenic transmission electron, and atomic force microscopy along with x-ray and neutron scattering have been applied to characterize the assembled structures.
C1.00050 Time-composition superpositioning in the rheological behavior of triblock copolymer/ selective co-solvent blends, ARJUN KRISHNAN, North Carolina State University, RUDOLF BUKOVNIK, Tyco Electronics Corp., RICHARD SPONTAK, North Carolina State University — Thermoplastic elastomers composed of styrenic triblock copolymers are of great importance in applications such as adhesives and vibration dampening due to their resilience and facile processing. The swelling of these polymers by adding midblock selective solvents or oligomers provides an easy route by which to modify the morphology and mechanical behavior of these systems. In this study we consider a ternary blend of a poly(styrene-b-(ethylene-co-butylene)-b-styrene) triblock copolymer and mixtures of two midblock selective co-solvents: a mineral oil that is liquid at ambient temperature, and a glassy tackifier resin that exhibits limited solubility in the midblock matrix. We use dynamic rheology to study the viscoelastic response of a wide variety of systems under oscillatory shear. The copolymer concentration is varied between 15 to 35 wt%, while the resin/oil ratio in the midblock-solvent matrix is independently varied. Frequency spectra acquired at ambient temperature display viscoelastic behavior that shifts in the frequency domain depending on the resin/oil ratio. At high oil loadings, the materials behave as physical gels. For each copolymer concentration, all the frequency data can be shifted by time-composition superpositioning to yield a single master-curve.

C1.00051 Drop shape analysis of poly-styrene acrylic acid gradient copolymer at oil/ water interfaces, WA YUAN, MICHELLE MOK, JOHN TORKELSON, KENNETH SHULL, Northwestern University — The behavior of poly-styrene/ acrylic acid gradient and block copolymers at liquid/liquid interfaces was investigated using drop shape analysis. Copolymers were dissolved in chloroform and then pendant drops of the solutions were created in water. The drop shape was monitored as a function of time in order to determine interfacial parameters. Molecular movements at the interface were inferred by measuring changes in interfacial pressure as the interface was contracted and expanded through control of the drop volume. A picture of the interfacial structure of gradient copolymer system was obtained from an analysis of these results. This analysis suggests that gradient copolymers are more interfacially active than block copolymers. The interfacial properties depend more strongly on the hydrophilic/hydrophobic ratio and sequence distribution than on the molecular weight.

C1.00052 Influence of Binding Strength on the Structure of Supramolecular Polymer-Surfactant Complexes, MANESH GOPINADHAN, Department of Chemical Engineering, Yale University, EVAN BEACH, PAUL ANASTAS, Department of Chemistry, Yale University, CHINEDUM OSUJI, Department of Chemical Engineering, Yale University — Specific interactions between small molecule species and host binding sites on a polymer chain can be used to engineer supramolecular complexes which display liquid crystalline order. In particular, hydrogen bonding interactions represent a flexible platform for the creation of graft-copolymer like structures by the reversible, specific association of small molecules with complementary sites on the polymer backbone. We use hydrogen bonding between the imidazole termination of mesogenic species and the carboxylic acid groups of poly(acrylic acid) to form side-chain liquid crystalline polymers in solution and in the melt state. We investigate their phase behavior and binding using a combination of calorimetry (DSC), x-ray scattering (SAXS), infrared spectroscopy (FTIR) and optical microscopy. We find that there is a critical interaction strength and critical stoichiometry required for the formation of a liquid crystalline mesophase in these systems. The manipulation of the binding equilibria via temperature makes for an interesting class of stimuli responsive materials in solution and in the melt state.

C1.00053 Registration of Lamellar Microdomains of PS-b-PMMA to Topographic Guiding Patterns, SANG-MIN PARK, CHARLES RETTNER, JED PITTERA, HO-CHEOL KIM, IBM Almaden Research Center — In addition to the control over orientation and lateral alignment, the control over precise placement of microdomains is critical for block copolymer lithography. We report here an approach for spatial registration of the lamellar microdomains of poly(styrene-b-methy methacrylate) (PS-b-PMMA) using topographic guiding patterns prepared by E-beam lithography. By employing two levels of topographic patterns, we could achieve both alignment and registration of lamellae on surface. Details on the limitations and challenges of this approach will be addressed along with potential applications to device fabrications. A mean field Monte Carlo simulation on an IBM BlueGene/L which provides additional structural insights into the influence of the topographic guiding patterns will be presented as well.

C1.00054 The Assembly of Cyclopeptide-Polymer Conjugates and Block Polymer, NANA ZHAO, Department of Materials Science and Engineering, University of California, BRETT HELMS, Material Sciences Division, Lawrence Berkeley National Laboratory, TING XU, Materials Science and Engineering, Department of Chemistry, University of California, Material Sciences Division, Lawrence Berkeley National Laboratory — The co-assembly of cyclopeptide-polymer conjugates and block polymer affords a simple route to generate hierarchical structures with molecular level control over the assemblies. By coupling synthetic homopolymer to a preformed cyclic (D-alt-L)-R- octapeptide, a family of coil-ring-coil bioconjugates was synthesized. The controlled self-assembly of the conjugate leads to uniform nanoparticle structures, 2.5-3nm in height and 25-30nm in diameter. The assembly of blends of cyclopeptide-polymer conjugates and diblock copolymers provide a base to generate nanoporous materials and improve our understanding in the self-assembly of multi-component hybrid systems.

C1.00055 Block Copolymer Based Supramolecules for Organoelectronic, BENJAMIN RANCATORE, Department of Chemistry, UC Berkeley, SHIH-HUANG TUNG, Department of Materials, UC Berkeley, CLAYTON MAULDIN, Department of Chemistry, UC Berkeley, PAUL TILLBERG, Department of Materials, UC Berkeley, CLAIRE WOO, Department of Chemical Engineering, UC Berkeley, JEAN M.J. FRECHET, Department of Chemistry, UC Berkeley, TING XU, Department of Materials, UC Berkeley — Block copolymer (BCP)-based supramolecules present unique advantages over conjugated BCPs to fabricate functional devices such as OLEDs and photovoltaics. The self assembly of 5"-(3,7-diethylacyl)-5-(3-hydroxyphenyl)propyl]-2,2'5',2"'-quaterthiophene (4T) hydrogen bonded to the poly(4-vinylpyridine) (P4VP) block of polystyrene-b-poly(4-vinylpyridine) (PS-b-P4VP) BCP was studied in bulk and thin films. Lamellae-within-lamellae hierarchical structure was observed and can be macroscopically oriented at both length scales in thin films. Films of pure 4T, P4VP(4T) and PS-b-P4VP(4T) composites were investigated as organic field-effect transistors (OFETs). Phase behavior of blends of the BCP-based supramolecule and PCBM were also investigated to guide the fabrication of organic photovoltaics.

C1.00056 Chain Bridging in Semicrystalline Multiblock Copolymers, MANAS SHAH1, VENKAT GANESAN2, The University of Texas at Austin — The structure development in semicrystalline/rubbery multiblock copolymers involves complex interplay between two self-ordering mechanisms — microphase separation and crystallization of one of the components. Experiments have suggested connection between the mechanical properties and the molecular architecture of such linear copolymers, especially the role of bridging conformations in multiblock copolymers. We present a theoretical study to evaluate the bridging/looping fractions in these multiblock copolymers as a function of the morphology and the molecular architecture. We model the non-crystalline (rubbery) component as a flexible Gaussian chain and the crystalline component as a semiflexible chain with a temperature dependent rigidity and a favorable tendency to form parallel bonds. We calculate the domain spacing in lamellar phases of diblock copolymer where one flexible chain is attached to the semiflexible chain and compare the scaling exponents with existing scaling theories for semicrystalline diblock copolymers. Using self-consistent field theory, the bridging fractions of the various domains in these complex multiblock copolymers (triblock and pentablock) are evaluated as a function of the sequence of the chains and other parameters in the system.

1 Graduate Student
2 Associate Professor
C1.00057 Tuning the Structure-Directing Block in Crystalline-Crystalline Diblock Copolymers, SHENG LI, SASHA MYERS, RICHARD REGISTER, Princeton University — Crystalline-crystalline block copolymers containing two or more chemically distinct crystallizable blocks are fascinating because their solid-state structures can be set either by block incompatibility or by crystallization of one or more blocks, depending on macromolecular design and processing history. Double-crystalline diblock copolymers of linear polyethylene (LPE) and hydrogenated polyboronene (hPBN) were synthesized, and their crystallization behavior and morphology were examined using two-dimensional simultaneous time-resolved synchrotron small-angle and wide-angle x-ray scattering. In previous work (Macromolecules 2008, 41, 6773), we showed that for diblock molecular weights of 50 kg/mol and above, the hPBN block always crystallized first and set the solid-state microstructure. In the present work, we explore the difference in molecular weight dependence of the melting/freezing points of LPE vs. hPBN to create materials where LPE is the structure-directing (templating) block. In 20 kg/mol diblocks, LPE block crystallizes first, even when LPE is the minority component, and restricts hPBN to crystallize between the LPE lamellae. In hPBN-rich diblocks, LPE crystallization triggers hPBN crystallization and the two blocks crystallize at almost the same rate. During cooling to room temperature, hPBN transitions from a rotationally disordered pseudohexagonal phase to a monoclinic structure.

C1.00058 Tethered Polyhedral Oligomeric Silsesquioxane on Lamellar Single Crystal of Poly(D-lactide), XIN-FEI YU, WEN-BIN ZHANG, RYAN VAN HORN, RODERIC QUIRK, STEPHEN CHENG, University of Pennsylvania — We report the synthesis and characterization of two copolymers having imidazolium based-ionic groups on POSS. The synthesis involved anionically polymerizing Poly(ethylene oxide)-b-poly(n-butyl methacrylate-r-3-trimethylsilylprop-2-ynyl methacrylate) block copolymer on a POSS-functionalized surface. The POSS-functionalized microdomains of the block copolymer were confirmed by small angle x-ray scattering (SAXS) and transmission electron microscopy (TEM). Tethering density of POSS was controlled by the molecular weight of PDLLA crystalline chain and by the variation of preparation conditions. Tethering density was increased as molecular weight of PDLLA was lower and crystallization temperature was increased higher.

C1.00059 A simple method to control the porosity in thin block-copolymer films, WONJOO LEE, XIN ZHANG, ROBERT M. BRIBER, University of Maryland, College Park — We report a simple way developed to control the porosity in block-copolymer films. PS-P4VP block copolymer/PS4VP homopolymer was dissolved at 80 °C for 12 hours and cooled to room temperature. Depending on the amount of PS4VP homopolymer, from 1% to 25% of PS4VP, the thin films prepared showed different morphologies depending on the composition of the material and the surface/substrates used. The films were examined by AFM and TEM. Interestingly, large scale macrophase-separation was not found regardless of the ratio of PS4VP and PS. Instead, it was found that microphase-separation occurred during the spincoating process for all concentrations of PS4VP homopolymer studied. The size of the microphase-separated domains increased as the ratio of PS4VP to PS increased, indicating that the added PS4VP homopolymer was contained within the P4VP microdomains. The PS-P4VP/P4VP blend films were then immersed for 3 hours in ethanol which induced a reconstruction of the film structure and removed the PS4VP homopolymer. The resulting morphology exhibited nanoscale porosity with the pore size increasing with increasing concentration of P4VP homopolymer. A possible mechanism for the microphase-separation for the formation of the nanoporous structure will be discussed.

C1.00060 Nanoscale functionalized surface pattern by combining block copolymer template and click chemistry, XINYU WEI, WEI CHEN, THOMAS RUSSELL, Univ of Massachusetts Amherst — Poly(ethylene oxide)-b-poly(n-butyl methacrylate-r-3-trimethylsilylprop-2-ynyl methacrylate) block copolymer was successfully prepared by atom transfer radical polymerization (ATRP) starting from a PEO macroinitiator, with good control of molecular weight, polydispersity and comonomer composition. The trimethylsilyl protecting group can then be quantitatively converted to terminal alkyne groups under mild conditions. Microphase separation of these block copolymers has been confirmed by small angle X-ray scattering (SAXS). Orientation of microdomains in thin films can be controlled by thermal or solvent annealing. Nanoparticles or biological macromolecules can be selectively immobilized onto the methacrylate microdomains through the cycloaddition between terminal alkynes and azides, which leads to a functionalized surface pattern for many applications.

C1.00061 Controlled morphology of Nafion® perflourinated ionomer membrane and poly(vinylidene-co-trifluoroethylene) blends for swelling suppression, NADZRNAHAMIN AHMAD NAZIR, THEIN KYU, University of Akron — The major objective of the present study is concerned with the swelling suppression of Nafion® membrane upon hydration through blending with poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) copolymer. The phase diagram of the Nafion/PVDF-TrFE blend was established by differential scanning calorimetry, cloud point measurement, and optical microscopy. A theoretical phase diagram was calculated by self-consistently solving the combined Flory-Huggins free energy for liquid-liquid demixing and the phase field free energy for crystal solidification. The resulting phase diagram is the combined LCST-UCST and/or an hour glass guide. Based on the phase diagram, the phase separated domain morphology can be controlled to exhibit bicontinuous or dispersed domains via phase separation by solvent casting or thermal quenching. The blends thus prepared not only afford suppression of water uptake, but also can maintain dimensional stability. Fourier transform infrared spectroscopy studies and water uptake measurements showed infallible evidence that modification of Nafion® with PVDF-TrFE reduces swelling upon hydration.

C1.00062 Synthesis and Morphology Study of Copolymers Containing Imidazolium Group, DAVID SALAS-DE LA CRUZ, University of Pennsylvania, SHARLENE R. WILLIAMS, JOHN LAYMAN, MATT GREEN, TIMOTHY E. LONG, Virginia Tech, KAREN I. WINEY, University of Pennsylvania — We report the synthesis and characterization of two copolymers having imidazolium based-ionic groups located either in the backbone or side chain. Imidazolium ionene segmented block copolymers, containing imidazolium group in the backbone, were synthesized from 1,1’-(1,4-butanediyl)bis(imidazole), 1,12-dibromododecane hard segments, and PTMO dibromide. Vinyl imidazolium random copolymers, containing the imidazolium group in the side chain, were synthesized from 1-butyl-bromide and 3-vinylimidazolium in ethyl acetate and copolymerized with methylmethacrylate. The morphological studies of micelles and nanofibers were performed through blending with poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) copolymer. The phase diagram of the Nafion/PVDF-TrFE blend was established by differential scanning calorimetry, cloud point measurement, and optical microscopy. A theoretical phase diagram was calculated by self-consistently solving the combined Flory-Huggins free energy for liquid-liquid demixing and the phase field free energy for crystal solidification. The resulting phase diagram is the combined LCST-UCST and/or an hour glass guide. Based on the phase diagram, the phase separated domain morphology can be controlled to exhibit bicontinuous or dispersed domains via phase separation by solvent casting or thermal quenching. The blends thus prepared not only afford suppression of water uptake, but also can maintain dimensional stability. Fourier transform infrared spectroscopy studies and water uptake measurement showed infallible evidence that modification of Nafion® with PVDF-TrFE reduces swelling upon hydration.

C1.00063 Nanoscale Ionic Aggregate Morphology in Zwitterionic Copolymers, JAE-HONG CHOI, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6722, REBECCA HUYCK, Department of Chemistry, Virginia Tech, Blacksburg, VA 24061, DAVID SALAS-DE LA CRUZ, University of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, Pennsylvania 19104 — The morphology of two different zwitterionic copolymers, poly(sulfobetaine methacrylate-ran-butyl acrylate), and poly(sulfobetaine methacrylamide-ran-butyl acrylate) are investigated as a function of the mol % content of SBMA (7 and 9 mol %) and SBMAm (6, 10 and 13 mol %), respectively. In both copolymers, X-ray scattering results show a new structure in the material arising from ionic aggregates. The sizes of the ionic aggregates are obtained through the scattering model. The sizes of the ionic aggregates increase as the ion content increases. The application of scanning transmission electron microscopy to the study of ionomer morphology has enabled direct, model-independent visualization of the ionic aggregates. The correlation between X-ray scattering results and the real space imaging for morphology of these zwitterionic copolymers will be presented.
C1.00064 Dynamics and Morphology of Sulfonated Polystyrene Ionomers by Dielectric Spectroscopy, ALICIA CASTAGNA, Penn State University, WENQIN WANG, KAREN I. WINEY, University of Pennsylvania, JAMES RUNT, Penn State University — The dynamics of sulfonated polystyrene (SPS) ionomers, in both the acid and neutralized forms, were investigated using broadband dielectric spectroscopy. The influences of acid content, counterion type (Zn, Na, and Cs), degree of neutralization, and microphase separated morphology on segmental and local dynamics, as well as on Maxwell – Wagner – Sillars interfacial polarization, were examined.Ionomers prepared from SPS containing 1.9 mol% sulfonic acid species exhibit a broader segmental process indicative of a considerably broader distribution of local environments, as compared to those in neutralized SPS. Moreover, multiple segmental relaxations were identified in the dielectric spectra of Zn and Na neutralized SPS (1.9 mol%) ionomers, likely indicating two distinct environments arising from ion clustering. A combination of STEM imaging and X-ray scattering confirmed the presence of monodisperse spherical ionic aggregates that were homogeneously distributed in the polymer matrix.

C1.00065 Dynamics of Strongly Associating Polymer Blends Using Broadband Dielectric Spectroscopy1, KEVIN MASSER, JAMES RUNT — In this study we investigate the dynamics of miscible polymer blends that preferentially form strong intermolecular hydrogen bonds. Random copolymers of p-(hexafluoro-2-hydroxyethyl-2-propyl)styrene [HFS] and 2,3-dimethylbutadiene [DMB] were synthesized for this study, as was the HFS homopolymer. HFS units are capable of forming strong intermolecular hydrogen bonds with complimentary species on a second miscible polymer, while minimizing the extent of intramolecular associations. The copolymers/homopolymers were blended with select homopolymers that form intermolecular hydrogen bonds of varying strength. Broadband dielectric relaxation spectroscopy is used to study segmental and local blend dynamics, which are observed to vary significantly in the presence of hydrogen bonding. Fourier transform infrared spectroscopy was used to determine the degrees and strengths of hydrogen bonding present in the blends.

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C1.00066 Investigating void development in filled elastomers under uniaxial strain, AILISH O’HALLORAN, National University of Ireland Galway, ARTHUR SCHOLZ, University of California Santa Barbara, KRISTIN SCHMIDT, University of California Santa Barbara, LIXIA RONG, Brookhaven National Laboratory, SHIGEYUKI TOKI, BENJAMIN HSIAO, Stony Brook University, ED KRAMER, University of California Santa Barbara — Development of voids during cyclic, uniaxial extension and retraction, of both silica and resin filled elastomers, was studied by combining synchrotron-based time resolved small angle X-ray scattering (SAXS) and primary X-ray beam attenuation with stress-strain curves measured simultaneously. These data were used to calculate the volumetric voids due to the development of voids during extension and their subsequent disappearance during retraction as well as the size and shape of the smaller voids. Four samples were investigated, one silica-filled polydimethylsiloxane (PDMS), one resin filled PDMS, and two silica filled polyphenylethylmethylsiloxane (PPMS), all candidate materials for dielectric elastomer actuators, in which void development would lead to decreased dielectric breakdown electric fields and premature failure.

C1.00067 Probing the Mullins Effect in Filled Elastomers by Small Angle X-ray and Neutron Scattering, ARTHUR SCHOLZ, Materials Department, UCSB, REX HJELM, MARK TAYLOR, Los Alamos Neutron Science Center, ED KRAMER, Materials Department, UCSB — While there has been considerable effort made to understand and model the effect that filler particles have on the mechanical properties of filled elastomers, the origins of a striking characteristic strain softening known as the Mullins Effect are still debated. Several micro-mechanical models have been proposed using a variety of mechanisms to describe the polymer-filler and filler-filler interactions to fit mechanical test data without any direct observation of microstructural changes. Small angle X-ray and neutron scattering provide complimentary methods for observing these changes on the relevant length and time scales necessary for identifying and characterizing the proposed mechanisms. We designed and built a modular uniaxial load frame for use in a variety of lab and user facilities. Its capabilities include a 350mm of symmetrical travel and a non-contact strain measurement system using speckle pattern digital image correlation. The system was developed and tested silica-filled polydimethylsiloxane (PDMS) and polyphenylethylmethylsiloxane (PPMS) elastomers using the Low Q Diffractometer at the Los Alamos Neutron Science Center at Los Alamos National Laboratory.

C1.00068 Segmented polyurethanes containing carbon nanotube nanohybrid shishkebabs, MATTHEW HOOD, Drexel University, JAMES SANDS, JOHN LASCALA, RICR BLEYER, Army Research Labs, CHRISTOPHER LI, Drexel University — Segmented polyurethanes (SPUs) are linear, multiblock copolymers that possess a wide range of tailorable properties via control during synthesis and processing. Phase separation between SPU’s segments produce superior elastomeric properties with hard domains maintaining the polymer matrix under stress, while soft domains provide flexibility allowing for a high degree of strain. We have synthesized a variety of SPU systems using different molecular weight macrodiol soft segments and various concentrations of hard segments, which are composed of hexamethylene disocyanate and butanediol. SPU morphology control via tuning the hard/soft segment ratio was achieved. Furthermore, adding carbon nanotubes (CNTs) that have been periodically patterned with functionalized crystalline polymers to the shishkebab hard segments and various CNT concentrations led to tunable mechanical properties of our SPU system even at low CNT concentrations. Differential scanning calorimetry, dynamic mechanical analysis, wide angle X-ray diffraction and transmission electron microscopy have been used to characterize these systems and compare them to neat SPU. By tailoring SPU composition and shishkebab concentration we have produced a system with significant mechanical improvement with potential for use as a shape memory polymer.

C1.00069 Efficient Synthesis of Poly( hydroxyethyl Methacrylate)-b-Poly(dimethyaminoethyl Methacrylate) Block Copolymer by Atom Transfer Radical Polymerization, WEI TANG, YUEH-LIN LOO, Engineering Quadrangle, Princeton University, Princeton, NJ 08544-5263 — Polymers containing hydroxyethyl methacrylate (HEMA) and dimethyaminoethyl methacrylate (DMEA)A have found wide applications in areas such as bioseparation, tissue engineering and controlled drug delivery. The controlled synthesis of block copolymers of PDMAEMA-b-PHEMA from PDMAEMA macronitiator by atom transfer radical polymerization (ATRP), however, has not been successful due to the loss of chain end functionality during polymerization. We report an ATRP system that affords efficient chain extension from PDMAEMA to HEMA using Cu(0)/1,1,4,7,10,10-hexamethyldiepoxynorprene as the catalyst, 2-chloropropionitrile as the initiator in methanol at room temperature. A clear peak shift in the gel permeation chromatography trace towards shorter elution times indicates chain growth on HEMA addition. The chain end functionalities of PDMAEMA are thus retained and can be used to efficiently initiate chain extension reaction of HEMA. This new synthetic route opens new possibilities for the synthesis of pH- and temperature-responsive systems containing DMAEMA.

C1.00070 Atom Transfer Radical Copolymerization of Gradient Copolymers of HEMA/DMAEMA with Arbitrary Composition Profiles, KEITH GALLOW, YUEH-LIN LOO, Princeton University — Gradient copolymers represent a new class of statistical copolymers where a non-uniform composition profile is controllably introduced along the length of the polymer chain. Gradient copolymers have thermal and mechanical properties that are different from random or block copolymers having the same average composition. Due to synthetic limitations, however, the introduction of arbitrary composition profiles remains challenging. Here, we demonstrate the ability to controllably introduce arbitrary composition profiles along copolymers of 2-hydroxyethyl methacrylate (HEMA) and 2-(dimethylamino)ethyl methacrylate (DAMAEMA) by atom transfer radical copolymerization in a semi-batch reactor. Using gas chromatography to monitor monomer consumption, respectively, and both show good agreement with our model’s predictions.
C1.00071 Improving the Electrical Conductivity of Polyaniline Through Molecular Control. JOUNG EUN YOO, WILLIAM KRÄKELBERG, TRACY BUCHOLZ, THOMAS TRUSKETT, YUEH-LIN LOO, PRINCETON UNIVERSITY TEAM, UNIVERSITY OF TEXAS AT AUSTIN COLLABORATION — We have investigated the electrical conductivity of polyaniline (PANI) that is template synthesized with a polymer acid of poly(2-acrylamido-2-methyl-1-propanesulfonic acid), PAAMPSA. The conductivity of PANI-PAAMPSA is determined by the particle density when PANI-PAAMPSA is cast as films. The PANI-PAAMPSA particle density can in turn be tuned by manipulating the molecular characteristics of PAAMPSA. Specifically, templating aniline polymerization with a higher molecular weight PAAMPSA results in bigger PANI-PAAMPSA particles; templating aniline polymerization with a broader molecular weight distribution PAAMPSA results in particles with a larger size distribution. The conductivity of drop-cast films of PANI-PAAMPSA therefore depends on how the particles pack in the solid state. In particular, we find the conductivity of PANI-PAAMPSA to increase with particle density. Additionally, PANI is preferentially segregated to the surface of these particles. The conductivity of PANI-PAAMPSA thus scales superlinearly with the surface area per unit volume of the cast film.

C1.00072 An Investigation of Polyelectrochromism in Water-Dispersible Polyaniline. JACOB TARVER, JOUNG EUN YOO, YUEH-LIN LOO, Department of Chemical Engineering, Princeton University — The promise of polyaniline (PANI)-based devices, such as electrochromic windows or billboards, is motivated by the coupled nature of PANI’s redox and chromic properties. In its fully reduced and oxidized form, PANI is electrically insulating and characteristically transmits yellow and violet, respectively. Protonation of PANI’s intermediate oxidation state induces electrical conductivity and shifts its transmission to green. This proton dependence has historically limited the use of small molecule acid doped PANI to acidic media. Template synthesis of PANI on poly(2-acrylamido-2-methyl-1-propanesulfonic acid), or PAAMPSA, yields electrostatically stabilized PANI-PAAMPSA particles; films comprising these particles maintain electroactivity in solutions as high as pH 10. Exposure to dichloroacetic acid moderates the electrostatic interactions, thereby relaxing the material’s global structure. This structural rearrangement significantly improves the stability and reversibility of repeated cycling between PANI’s redox states. Relaxation of PANI-PAAMPSA’s structure thus affords enhanced robustness to this readily-processible system.

C1.00073 Development of Polymer Electrolyte Membrane (PEM) from Bisphonol S for Direct Methanol Fuel Cell (DMFC). SAIRUNG CHANGKHAMCHOM, ANUVAIT SIRIVAT TEAM — The currently used Proton Exchange Membrane (PEM) in a Direct Methanol Fuel Cell (DMFC) is Nafion®, an excellent proton conductor in a fully hydrated membrane. However, it has major drawbacks, such as very high cost, and loss of conductivity at elevated temperature and low humidity. In this work, a novel PEM based on sulfonated poly(ether ether ketone) (S-PEEK). Poly(ether ether ketone) (PEEK) was synthesized by the nucleophilic aromatic substitution polycondensation of Bisphonol-S and 4,4’-difluorobenzophenone for system A, and Bisphenol S and 4,4’-dichlorobenzophenone for system B. Bisphenol-S helps to increase the thermal stability due to its high melting point (245°C). The post-sulfonation reaction was performed by using concentrated sulfuric acid. Sulfonated poly(ether ether ketone) (S-PEEK) samples were characterized by FTIR and 1H-NMR to confirm the chemical structure of the S-PEEK, and by TGA to investigate the thermal property.

C1.00074 Iontophoresis of Salicylic Acid From Salicylic Acid Doped Poly(p-phenylene vinylene)/Polyacrylamide Hydrogels. SUMONMAN NIALLANG, ANUVAIT SIRIVAT TEAM — The apparent diffusion coefficients, D_app, and the release mechanisms of salicylic acid from salicylic acid-loaded polyacrylamide hydrogels, SA-loaded PAAM, and salicylic acid-doped poly(p-phenylene vinylene)/polyacrylamide hydrogels, SA-doped PPV/PAAM, were investigated. In the absence of an electric field, the diffusion of SA from the SA-doped PPV/PAAM hydrogel is delayed in the first 3 hr due to the ionic interaction between the anionic drug and PPV. Beyond this period, SA can diffuse continuously into the buffer solution through the PAAM matrix. D_app of SA-doped PPV/PAAM is higher than that of the SA-loaded PAAM, and the former increases with increasing electric field strength due to the combined mechanisms: the expansion of PPV chains inside the hydrogel; iontophoresis; and the electroporation of the matrix pore. Thus, the presence of the conductive polymer and the applied electric field can be combined to control the drug release rate at an optimal desired level.

C1.00075 Morphology of Hole Injection Layers for Polymer Light Emitting Diodes. KRISTIN SCHMIDT, KAREN E. SOHN, Materials Research Laboratory, University of California, Santa Barbara, FABRICE AMY, LING YANG, Air Products and Chemicals Inc, Pennsylvania, EDWARD J. KRAMER, Materials Research Laboratory, University of California, Santa Barbara — Hole injection layers (HIL) play important roles in improving the device efficiency and stability of polymer light emitting diodes (PLED) as they can enhance the hole injection from the ITO electrode. It was shown that thermal annealing of the PLEDs results in a remarkable improvement in the long-term stability of the device. These reports lead to the hypothesis that changes in the morphology of the phase separated mixture of the polymers in the HIL is responsible for this improvement. However, no experimental evidence of such morphological changes exists. To investigate the morphological changes during annealing we performed NEXAFS, SAXS and GISAXS experiments on thin films of different blends consisting of poly(3,4-ethylene dioxythiophene) (PEDOT) with either poly(fluoroethylene-r-fluoroether-ether ketone) (S-PEEK). Poly(ether ether ketone) (PEEK) was synthesized by the nucleophilic aromatic substitution polycondensation of Bisphonol-S and 4,4’-difluorobenzophenone for system A, and Bisphenol S and 4,4’-dichlorobenzophenone for system B. Bisphenol-S helps to increase the thermal stability due to its high melting point (245°C). The post-sulfonation reaction was performed by using concentrated sulfuric acid. Sulfonated poly(ether ether ketone) (S-PEEK) samples were characterized by FTIR and 1H-NMR to confirm the chemical structure of the S-PEEK, and by TGA to investigate the thermal property.

C1.00076 Nanoparticle Tethered Perylene Tetracarboxylic Diimides as Novel Photo Harvesting Antennae. WENBIN ZHANG, BIN SUN, HUI LI, MATTHEW PANZNER, WILEY YOUNGS, RODERIC QUIRK, STEPHEN CHENG, Maurice Morton Institute and Department of Polymer Science, Department of Chemistry, The University of Akron — Shape-persistent, well-defined, incompressible nano objects, such as polyhedral oligomeric silsequioxane (POSS) and C60, have been connected covalently to perylene tetracarboxylic diimide (PDI) to give a series of nanoparticle tethered PDI molecules, which could self-assemble into various ordered structures. For example, POSS end-capped PDI, namely POSS-PDI-POSS, grows single crystal lamellae of dimensions up to the centimeter scale in length. The crystal structure has been determined to be triclinic with a = 1.14 nm, b = 2.09 nm, c = 2.31 nm and α = 89.9°, β = 81.9°, γ = 82.3°. It shows that POSS forms bilayers in the crystal separated by PDI dimer molecular planes along the c axis. The self-assembly of the asymmetric POSS-PDI-C60 is even more intriguing. It gives single crystals with alternating POSS and C60 layers separated by PDI planes, which holds promising applications as photo harvesting antennae in photovoltaics. Our results show that nanoparticles could interplay with the strong p-p interaction and assist the self-assembly to ordered structures.
C1.00077 Highly Ordered Phases in Electrochemically Deposited Poly(3,4-ethylenedioxythiophene) (PEDOT)—LiBr\(^1\). JINGHANG WU, SARAH SPANNINGA, DAVID MARTIN, University of Michigan — Poly(3,4-ethylenedioxythiophene) (PEDOT) is a widely used \(\pi\)-conjugated polymer of considerable current interest for a variety of different applications such as biosensors, antireflective layers, electroluminescent devices, and hole injection layers in organic light emitting diodes and photovoltaics. These films have high conductivity, as well as thermal and chemical stability. PEDOT films prepared by chemical or electrochemical polymerization with different counter ions have shown different levels of modest order and crystallinity, typically with limited molecular orientation and relatively small crystallites. We have developed methods for preparing highly ordered phases by the electrochemical polymerization of PEDOT onto polycrystalline conducting substrates with LiBr as the counterion. The polymerizations are conducted at room temperature from aqueous solution. These phases have ordered crystalline domains that are hundreds of microns in size, and are uniformly birefringent. The structure of the ordered phase was characterized by optical and electron microscopy, X-ray diffraction, as well as infrared and X-ray photoelectron spectroscopy.

\(^1\)National Science Foundation

C1.00078 Sensitivity Enhancement of PEDOT-PSS towards CO by Zeolite ZSM-5 Additive. POJJAWAN CHANTHAANONT, ANUVAT SIRIVAT TEAM\(^1\) — Polymer-based gas sensors have received considerable interest in recent years, due to their gas sensing ability through the electrical conductivity changes when exposed to gases. In our research, poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonic acid), PEDOT-PSS, was synthesized via the oxidative polymerization and zeolites were used as selective microporous adsorbent to improve selectivity and sensitivity of the sensors. PEDOT-PSS were fabricated with zeolites by dry mixing and compressed to form PEDOT-PSS/zeolite composites. Zeolites ZSM-5 were chosen to investigate the effect of Si/Al mole ratios of zeolite on the electrical conductivity sensitivity response of PEDOT-PSS,1,1/zeolite ZSM-5 composites when exposed to CO. The electrical conductivity sensitivity of PEDOT-PSS,1,1/zeolite composites towards CO negatively increases with decreasing Si/Al mole ratios of zeolite ZSM-5. The highest electrical conductivity sensitivity response is obtained from PEDOT-PSS,1,1/Zeolite-ZSM-5(Si/Al = 23).

\(^1\)Corresponding Author

C1.00079 Flexible Field Emission Devices\(^1\), SUNNY SETHI, ALI DHINOJWALA, THE UNIVERSITY OF AKRON TEAM — We report synthesis of flexible field emission devices using patterned and non-patterned vertically aligned carbon nanotube arrays and use of such devices to induce phosphorescence. Carbon nanotube is known to have excellent electron emitting properties. On macroscopic scale, emission current density is much less than that for a single nanotube for reasons like screening effect and non uniform emission. Here, we report a very unique way to fabricate flexible field emission devices using partially entrapped aligned nanotubes in an elastomer as cathode. Using this process not only helps in fabricating a flexible geometry but also helps in the reduction of screening effect, thus increasing the emission efficiency. Emission current for these devices was studied with respect to the area and total perimeter for patterned nanotubes. These studies help to understanding the mechanism to translate nanoscopic emission to a macroscopic scale.

\(^1\)Funded by National Science Foundation

C1.00080 Effect of light attenuation on motion of photo-responsive polymer gels. PRATYUSH DAYAL, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Nature has found an efficient way to utilize chemical reactions to produce mechanical work. Whenever the need for energy arises, the chemical reactions in our body produce energy, which is used to generate mechanical response. Scientists have been trying to replicate the same functionality in man-made systems. One of the recent approaches couples the Belousov-Zhabotinsky (BZ) reaction and the mechanical properties of the gel to produce self-sustained oscillations. To study the effect of light on the mechanical behavior of the gel, we use our recently developed 3D gel lattice spring model (gLSM) which couples the BZ reaction kinetics to the gel dynamics. In order to include the effect of the polymer on the reaction kinetics, the Oreganator model for the photo-sensitive BZ reaction was modified. Using modeling and simulations, we have been able to control gel's shape and its locomotion using light as an external stimulus. Here we show that the intrinsic non-homogeneity in light intensity, created by gel can induce autonomous motion of the gel away from light.

C1.00081 Watching Nanoparticles Move through Polymers, JUAN GUAN, BO WANG, STEPHEN ANTHONY, SUNG CHUL BAE, STEVE GRANICK, U of Illinois - Urbana - Champaign — Several recent experiments show that the Stokes-Einstein equation used to describe particle diffusion is violated when nanoparticles are surrounded by polymer chains. In some systems, particles move faster; in others, more slowly, depending on the size of the probe. It is generally agreed that the relative timescale for a polymer chain to relax and a nanoparticle to diffuse the size of a polymer chain are what matter. In this work, we embed fluorescently-labeled nanoparticles within polymer solutions and use single-particle tracking to understand the relative motions of the two. A unique aspect is that we track motions not just of the nanoparticles but also those of the polymer chains in which they are embedded. The worst-case resolution of 30 nm in nanoparticle relative position is improved when slow motions improve the signal-to-noise.

C1.00082 An emerging theoretical picture of yielding for entangled polymeric liquids undergoing sudden deformation and flow. SHI-QING WANG, University of Akron, P.E. BOUKANY, S. RAVINDRANATH, Y.Y. WANG, X. LI, University of Akron — Recent particle-tracking velocimetric observations coupled with conventional rheological measurements have offered us a window to peek into processes responsible for a whole family of phenomena in entangled polymeric liquids. At a high rate of deformation imposed suddenly, entangled liquids can only respond like a solid and must undergo yielding before eventual flow is to take place. Until recently, how such a yielding process produces the observed scaling characteristics of the stress overshoot has remained elusive. More surprising and perplexing to many is that an elastic yielding process can also occur after cessation of any further external deformation. These experimental observations have provided the essential ingredients in the emerging theoretical picture of polymer deformation and flow.

C1.00083 Gas Diffusion and Free Volume Behavior of Ethylene Vinyl Alcohol Copolymers: Effect of Hydrogen Bonding Interaction. JUSTIN BRANDT, SERGEI NAZARENKO, BRIAN OLSON, University of Southern Mississippi, ALEXANDER JAMESON, Case Western Reserve University — The main objective of this work was to develop fundamental understanding of oxygen transport in a broad range of EVOH copolymers as it is related to free volume characteristics and hydrogen bonding interaction. FTIR was used to directly characterize H-bonding network as a function of copolymer composition and temperature. Positron annihilation lifetime spectroscopy (PALS) was used to study free volume behavior. The measure of intermolecular interaction, cohesive energy density, was calculated through group contribution methods and also obtained using molecular dynamics computer simulations. Oxygen transport characteristics of the copolymers, i.e. permeability, diffusivity, and solubility were measured at various temperatures, and the apparent activation energy parameters calculated.
C1.00084 The Viscoelastic Bulk Modulus: Effect of Crosslink Density, JIAXI GUO, SINDEE SIMON, Department of Chemical Engineering, Texas Tech University — The pressure relaxation response is measured at various temperatures in the glass transition region for two polycyanurate networks of differing crosslink density using a pressurizable dilatometer. Master curves are formed by the time-temperature superposition theory using vertical shifts to account for the temperature dependence of the bulk moduli. The results show that the pressure relaxation response has a small dependence on the viscoelastic density of the polycyanurate. However, the horizontal and vertical shift factors show a similar dependence on temperature when plotted in the form of T* vs. Tg. The horizontal shift factors agree well with those from the shear viscoelastic response. The relaxation spectra obtained from the pressure relaxation measurements will also be compared to those from shear stress relaxation experiments, and the validity of Leaderman’s hypothesis that the bulk and shear responses arise from different molecular mechanisms will be discussed.

C1.00085 Adhesion Behavior of Non-planar Wrinkled Surfaces, SANTANU KUNDU, University of Massachusetts-Amherst, RAVI SHARMA, Bausch and Lomb Inc, ALFRED CROSBY, University of Massachusetts-Amherst — Topological patterns on polymer surfaces can be used to significantly alter the surface properties, such as adhesion and contact angles. Conventional patterning methods, including photo- and imprint lithography, are difficult to apply to non-planar surfaces. Surface wrinkling induced by swelling of a soft substrate constrained by a stiff, thin surface layer offers an attractive approach. Using this method, surface patterns of various length scales over a large area on curved geometries were obtained. Controlling the thickness of the stiff layer (silicate) on a soft foundation (polydimethylsiloxane elastomers) and the strain conditions, amplitude and wavelength of the wrinkles were varied. We quantified the effect of wrinkule morphology on the adhesion of non-planar substrates.

C1.00086 Microvoid formation and strain hardening in highly cross-linked polymer networks, DEBASHISH MUKHERJI, CAMERON ABRAMS, Drexel University — Highly cross-linked polymer (HCP) networks are becoming increasingly important as high-performance adhesives and multifunctional composite materials. Because of their cross-linked molecular architectures, HCP’s can be strong but brittle. One key goal in improving the performance of HCP is to increase their toughness without sacrificing their strength. We use molecular dynamics simulations to study the mechanical properties of HCPs. We observe strain hardening in HCP glasses under tension and deformation. We show that formation of micro-voids, without bond-breaking, constitutes the microscopic origins of strain hardening. Micro-void-based strain hardening is not observed in a separate model by imposing a tetrahedral bond angle constraints. Strain hardening makes HCP networks ductile, thus indicating that flexible cross-linkers may be a possible means to control toughness of an HCP without sacrificing its strength.

C1.00087 Quantification of Molecular and Nanostructural Topology, RAMNATH RAMACHANDRAN, University of Cincinnati, GREGORY BEAUCAGE, University of Cincinnati — We have recently derived a method for the description of complex molecular and nanostructural topologies based on a statistical analysis. The method has been applied to a wide range of materials from long chain branched polyolefins, hyperbranched polymers, star polymers, H-branched polymers to cyaclics, biopolymers, and branched nanostructured aggregates. This method, when applied to neutron scattering data from dilute polymer solutions, yields the mole fraction of a structure involved in long chain branching, the branching density, and the average branch length. Moreover, quantitative measures of the convolution or tortuosity of the structure and the connectivity of the molecules can be made, opening a new window for our understanding of complex molecular topologies. When applied to neutron scattering the approach is applied to the chain-scaling regime at low to moderate values of the scattering vector. At high scattering vector the Kuhn length is observed that has been shown to be directly related to short chain branching in polyolefins. By combining information of short and long chain branching a topological map of complex molecular structure becomes possible. The method is quite generally applicable. This understanding has recently been applied to model long-chain branched polyethylene.

C1.00088 Computer simulation study of solvent quality and reaction geometry on controlled radical polymerization, SALOMON TURGMAN, JAN GENZER, North Carolina State University — Bulk- and surface-initiated controlled radical polymerizations are simulated using a stochastic Monte Carlo algorithm by following the bond-fluctuation model scheme and an attractive potential acting among bonded monomer beads. Specifically, we investigated the changes in polymer molecular weight and molecular weight polydispersity index (PDI) due to conformational variations of the chains that occur upon altering solvent quality. Variations in reaction geometry, temperature, initial monomer and initiator concentration, probability of initiation, initial probability of monomer addition, probability of termination, fraction of living polymers and their lifetime were studied. Synergistic effects among these parameters and the geometry of the reaction were also explored. Preliminary results suggest that polymerization in poor solvent quality solvents result in shorter polymers and increased molecular weight PDI.

C1.00089 Borylation of Polystyrene: Random Blocky vs. Truly Random Copolymers, WAYNE POWERS, Rensselaer Polytechnic Institute, ZACHARIAH NORMAN, CHANG RYU, Rensselaer Polytechnic Institute, CHULSUNG BAE, University of Nevada - Las Vegas, JAN GENZER, North Carolina State University, WAYNE POWERS, ZACHARY NORMAN, CHANG RYU TEAM, CHULSUNG BAE COLLABORATION, JAN GENZER COLLABORATION — Borylated PS with tuned blockiness of borylated styrene segments has been synthesized in methycyclohexene, using a bis[pinacolato]diphenylborato(1-)ligand(1) dirhodium(I) dichloride as catalysts. By performing the borylation reaction below and above the theta temperature of PS in methycyclohexene, 70 degrees Celsius, the co-monomer sequence distribution in the borylated PS changed from random-blocky to random, respectively. The “chemicalcoloring” is carried out at low PS concentration in order to ensure that individual chains do not coagulate during the borylation at temperatures below the theta temperature. NMR, SEC, cloud point measurements, and adsorption-based interaction chromatography are used to characterize the properties of borylated PS and elucidate the effects of blockiness on solubility and surface adsorption.

C1.00090 Phase behavior study of polystyrene and deuterated polystyrene in alkyl-cyclohexanes, ZACHARIAH NORMAN, Rensselaer Polytechnic Institute, WAYNE POWERS, CHANG RYU, Rensselaer Polytechnic Institute, ZACHARIAH NORMAN, WAYNE POWERS, CHANG RYU TEAM — To advance the controlled chemical modification of polystyrene (PS) and deuterated polystyrene (DPS) in solution, the phase behavior of PS and DPS in alkyl-cyclohexane solvents has been studied. Cloud point measurements have been performed by a house-made turbidity instrument using a picolog thermistor and a laser with a photoelectric cell converted to interface with a picolog TH-03 three channel thermistor converter. Solution phase diagrams for molecular weights of PS varying from 67 thousand to 1.8 million have been presented for methyl cyclohexane, propyl cyclohexane, isopropyl cyclohexane, butyl cyclohexane and isobutyl cyclohexane for the measurements of critical solution temperatures as a function of molecular weight. The theta temperature of polystyrene in each of these solvents has been estimated through extrapolation from the molecular weight dependence of the critical temperatures from the cloud point measurements.

C1.00091 Zero-dimensional organic nanoparticles via copolymer directed self-assembly, DEQUAN XIAO1, KUNHUA LIN, Department of Chemistry, Sichuan University, Chengdu, 610064 China, QIANG FU, Department of Polymer Science and Engineering, Sichuan University, State Key Laboratory of Polymer Materials Engineering, Chengdu, 610065 China, QINJIAN YIN, Department of Chemistry, Sichuan University, Chengdu, 610064 China — Inspired by inorganic nanomaterials, low-dimensional organic nanostructures have emerged as a new field of nanomaterials with the presence of size-dependent physical properties. Here, we report a zero-dimensional organic nanoparticles formed by copolymer-directed self-assembly. The nanoparticles are thermally stable up to ~200°C. The nanoparticle morphologies are probed by TEM and SEM images. The quantum confinement effect is suggested by the appearance of strongly broadened Raman shift spectra. By proof-of-principle quantum chemical calculations, we suggested that both vibration-vibration and electron-vibration coupling at nanoscale can cause the Raman broadening. The present organic nanoparticles provides a new class of nanostructures to exploring size-dependent physical properties.

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C1.00092 Capillary thinning and break-up of hydrogel-elastomer composites, YINAN LIN, DARRELL RENEKER, The University of Akron — The development of a filament stretching rheometer with a high magnification and high speed digital imaging system enabled real-time video observation of the extensional behavior of the hydrogel-elastomer complex fluids. Under a motor-controlled process of tip-plate separation, ethanol solutions of polyurethane with superabsorbent particles, which can be electrospun into nanocomposite nanofibers, evolved in profile. The rapidly shrinking jet diameter was measured from video images. As in extensional rheology of homogeneous polymer solutions, the elongational viscosity and the relaxation time calculated from the time dependence of midpoint diameters define a two-dimensional operating diagram for capillary self-thinning and capillary break-up.


C1.00093 Ultrafast Nanocalorimetry and Superheating in Linear Polymers1, CHRISTOPH SCHICK, ALEXANDER MINAKOV, ANDREAS WURM, University of Rostock — To study phase transition kinetics on submillisecond time scale a set of new membrane gauges for ultrafast scanning nanocalorimetry were constructed. Controlled ultrafast cooling, as well as heating, up to 106 K/s was attained. The characteristic rate R0 corresponding to the quasi-static limit of the temperature change in the membrane-gas system was determined. The rate R0 equals 105 K/s for the different gauges in helium gas. The method was applied for the measurements of the superheating phenomenon in a set of linear polymers: IPP, PBT, PET, iPP. A power law relation between the superheating and the heating rate was observed in the broad range 10E-2 – 10E4 K/s of the heating rates. A limiting superheating of about 10% of the melting temperature was observed at rates above 10E4 – 10E5 K/s. This limit depends on the annealing conditions before the sample melting. The observed superheating limit, as well as the power law, can be accounted for the internal stresses induced by the superheating near the crystalline-amorphous interface in semicrystalline polymers, which are related to the thermal expansion gradients inherent for a semicrystalline material.

1 We gratefully acknowledge the support of DFG.

C1.00094 Intermolecular Interactions in Polymer/C60 Blends, PETER MIRAU, AFRL/RXBN, Air Force Research Lab, Bio-Nano Branch, Wright-Patterson AFB, OH 45433, MARJAN LYONS, Wright State University, Dayton, OH — Solid-state NMR and x-ray scattering are used to study intermolecular interactions in blends of C60 with polystyrene, poly(9-vinyl carbazole) and poly(ethylene oxide). Miscible C60 blends prepared by solution precipitation with polystyrene and poly(9-vinyl carbazole) are purple in color, show intermolecular C60-polymer cross polarization and do not show the scattering peaks from C60 crystallites. In contrast, phase separation is observed in poly(ethylene oxide) blends. The C60 dynamics in the miscible blends are measured using the chemical shift anisotropy filter NMR pulse sequence, and the results show that the C60 in the rotating rapidly enough at ambient temperature to average the 18 kHz-wide chemical shift anisotropy line shape. Blending with C60 has no effect on the polystyrene dynamics as measured by the carbon spin-lattice relaxation times but leads to a narrowing of the proton line shapes as measured by 2D wide line correlation NMR. These results show that C60 interacts weakly with polymers, and the implications for weak interactions between polymers and carbon nanotubes are considered.

C1.00095 Effect of Hydrophobicity on the Adsorption of Human IgG to Thiolated Gold Surfaces as Characterized by SPR, KRISTEN DUTHIE, ADELE POYNOR, Allegheny College Physics Department — In order to enhance our understanding of the role of hydrophobicity in nonspecific human immunoglobulin G [hIgG] surface interactions, we studied the adsorption of hIgG to thiol self-assembled monolayers [SAMs] on gold using surface plasmon resonance [SPR]. The hydrophilic and hydrophobic SAMs had hydroxyl and methyl terminal groups respectively. Protein adsorption to thiolated surfaces was measured looking at relative SPR resonance angles.

C1.00096 Understanding Rubber Friction in the Presence of Water Using Sum Frequency Generation Spectroscopy1, PING-YUAN HSU, KUMAR NANJUNDIAH, ALI DHINOJWALA — Infrared-visible sum-frequency-generation spectroscopy (SFG) was used to study the molecular structure of water between a poly (dimethylsiloxane)(PDMS) and a sapphire substrate. The observation of SFG peaks associated with the dangling surface hydroxyl groups (3690 cm−1) and water bands (3000-3400 cm−1) indicates that the contact spot between the PDMS lens and the sapphire substrate is heterogeneous. Within the contact spot are regions where the methyl groups of the PDMS chains are in direct contact with the surface hydroxyl groups on the sapphire substrate. In the other regions, a thin water layer is trapped between the two surfaces with spectral features that are different from that of the unconfined water next to the sapphire or the PDMS surface. The higher adhesion and friction values observed in these experiments are consistent with the hypothesis that the contact spot is heterogeneous. These results have important implications in understanding the sliding behavior of wet, deformable hydrophobic materials on hydrophilic substrates. We have extended this experimental technique to study oil/water/solid interfaces.

1 This work was supported National Science Foundation

C1.00097 Protected Plasmonic Nanostructures for High Resolution Chemical Imaging using Tip Enhanced Raman Spectroscopy, REBECCA BUTT, CARLOS BARRIOS, ANDREY MALKOVSKY, ALEXANDER KISLIUK, University of Akron, Dept of Polymer Science, ALEXEI SOKOLOV, University of Akron, MARJAN LYONS, Wright State University, Dept of Polymer Science — Tip enhanced Raman spectroscopy (TERS), an emerging technique that combines optical microscopy and scanning probe microscopy, provides the sensitivity and selectivity necessary for high-resolution chemical imaging of polymer surfaces. An unprecedented 20 nm lateral resolution for the chemical imaging has been achieved. Unfortunately, the fragile plasmonic structures used to enhance the electric field are prone to mechanical, chemical, and thermal degradation. Developing robust noble metal nanostructures with stable plasmonic resonance is essential to reliable high resolution chemical imaging. Covering the metal layer with organic and inorganic ultrathin coatings is being investigated to extend the plasmonic activity of the engineered nanostructures. Addition of an ultrathin aluminum oxide (Al2O3) coating to a silver-coated scanning probe microscopy tip for TERS significantly improves plasmonic structure stability without sacrificing the initial TERS efficiency. This ultrathin coating provides wear resistance and stops chemical degradation responsible for the loss of signal enhancement.

C1.00098 Infrared and optical spectroscopy study of UHMWPE polymers, M.S. WOLF, J.N. MORVAN, John Carroll University, S.V. DORDEVIC, The University of Akron, N. STOJILOVIC, John Carroll University — Ultra-High Molecular Weight Polyethylene (UHMWPE) is very often the material of choice for the bearing surfaces of most hip and knee implants primarily due to its low friction combined with good toughness and abrasion resistance. We investigate optical properties of biomedical-grade UHMWPE GUR 1020 powders and sheets using infrared and UV-vis spectroscopy and compare results with those from industrial grade samples. In addition, we use X-ray diffraction spectroscopy to monitor the changes in crystal structure of these polymers as a function of temperature. Finally, we deliberately oxidize and subsequently characterize these materials since the oxidation of UHMWPE bio-implants is believed to be responsible for their failure in vivo.

C1.00099 ABSTRACT WITHDRAWN
C1.00100 A spectroscopic ruler to measure chain conformations at the solid-liquid interface. SUBHALAKSHMI KUMAR, JANET WONG, SUNG CHUL BAE, STEVE GRANICK, Department of Material Science and Engineering, University of Illinois at Urbana-Champaign — There do not appear to exist prior measurements of the conformations of polymers adsorbed to dilute coverages at the solid-liquid interface, in spite of abundant theoretical predictions. Here direct information is obtained by monitoring the fluorescence energy transfer between dyes located at the two ends of adsorbed polymer chains. The basic idea is that the farther the chain ends are spaced, the less efficient, and slower, is energy migration between these dyes. It occurs on the nanosecond time scale and is measured here by time-correlated single photon counting. From corresponding experiments performed with the same polymer chains labeled at one sole end, the contribution of rate of energy transfer to rotational anisotropy is decoupled from intrinsic rotational motion of the dyes themselves.

C1.00101 Vibrational Relaxation and Dynamical Transitions in Atactic Polystyrene. HANQING ZHAO, YUNG PARK, PAUL PAINTER — Infrared bands and Raman lines recorded in the frequency domain have a counterpart in the time domain in the form of time-correlation functions, which are sensitive to molecular dynamics on the picosecond time scale. This is explored by calculating time correlation functions and their variation with temperature for the conformationally insensitive modes observed near 1601 cm-1 and 1583 cm-1 in the infrared spectrum of atactic polystyrene. The correlation functions were modeled by assuming that there is a fast relaxation process characterized by a single relaxation time that is inhomogeneously broadened by a slower process, also characterized by a single relaxation time. The fundamental mode, near 1583 cm-1, is inhomogeneously broadened, but the relaxation time calculated for this mode is sensitive to temperature as a result of anharmonic coupling to a combination mode. A change in the modulation in the 1583 cm-1 band becomes apparent about 10–20 degrees below the thermally measured Tg. Relaxation times at first increase then decrease and becomes negligible at temperatures near 180 degrees. These results are consistent with theories of the glass transition.

C1.00102 Specific Heat Spectroscopy of Simple Chain Models. JONATHAN R. BROWN, JOHN D. MCCOY, New Mexico Institute of Mining and Technology, DOUGLAS ADOLPH, Sandia National Laboratories, BRIAN BORCHERS, New Mexico Institute of Mining and Technology — Molecular dynamics simulations were run on bead-spring polymer models. Small amplitude temperature variations were imposed, and energy response was monitored. The real and imaginary components of the frequency dependent specific heat were extracted. A low frequency peak is seen to develop at high packing fractions. The non-Debye parameter – β – is seen to decrease as the glass transition is approached. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

C1.00104 Reversible hydrogen storage in LiBH4/CaH2 with NbF5. JAE-HAM LIM, JAE-HYEOK SHIM, YOUNG-SU LEE, YOUNG WHAN CHO, Korea Institute of Science and Technology. JOONHO LEE, Korea University — Reversible hydrogen storage properties of 6LiBH4 + CaH2 composite have been investigated. 6LiBH4 + CaH2 composite with catalytic additives have been prepared using high-energy ball milling. Among various catalytic additives, the addition of NbF5 exhibits the lowest dehydrogenation temperature. During dehydrogenation, this composite is decomposed into LiH and CaB6 releasing about 9 wt pct hydrogen. The van’t Hoff plot from the equilibrium pressures measured at different temperatures predicts that the equilibrium temperature under 1 bar of hydrogen is 582 K and the reaction enthalpy change is 56.5 kJ/mol H2. This is consistent with the results of thermodynamic calculation. Rehydrogenation of this composite is accomplished at 723 K under 100 bar of hydrogen after dehydrogenation, presenting a reversible hydrogen capacity of about 9 wt pct.

C1.00105 LiBH4+Ca(BH4)2 composite system for hydrogen storage. JI YOUN LEE, YOONYOUNG KIM, YOUNG-SU LEE, JAE-HYEOK SHIM, YOUNG WHAN CHO, Korea Institute of Science and Technology, Republic of Korea, DORTHE RAVNSBRO, TORBEN JENSEN, University of Aarhus, Denmark, NINGSER CERENIUS, Lund University, Sweden — LiBH4 is one of the promising candidates for hydrogen storage materials because of its high gravimetric and volumetric hydrogen capacity. However, dehydrogenation of LiBH4 occurs above 400°C, which limits its use in its pristine form. By mixing with Ca(BH4)2, we have tried to lower the dehydrogenation temperature. The underlying design principle of this composite system is the recently proven reversibility of 6LiBH4+CaH2 composite and Ca(BH4)2 itself. Using differential scanning calorimetry and in-situ synchrotron XRD measurement, we observed eutectic melting of (1-x)LiBH4 + xCa(BH4)2 at around 200°C in a wide range of x. The decomposition characteristics and the hydrogen capacity of this composite vary with x, and at a certain value of x we found that decomposition was finished below 400°C showing more than 10 wt% hydrogen capacity. Reversibility of this system was also confirmed.

C1.00106 Nonlinear thermoelectric behavior in double-barrier quantum-dots. ERIC HOFFMANN, NATTHAPON NAKPATHOMKUN, University of Oregon, HENRIK NILSSON, Lund University, ANN PERSSON, University of Oregon, LARS SAMUELSON, Lund University, HEINER LINKE, University of Oregon — Thermovoltage in bulk material systems is to good approximation linear in applied temperature difference, ΔT, with the constant of proportionality being the thermopower, S. However, this linear relationship does not necessarily hold true for nanoscale thermoelectrics[1]. Here we report on basic research which uses a simple quantum dot as an example nanoscale system for studying nonlinear thermoelectric phenomena. Specifically, we show experimentally as well as theoretically that strong modulations in the transmission function of the quantum dot manifests into thermovoltages and thermocurrents which are not linear in ΔT at ΔT as small as ΔT/T = 0.1. Quantum-dot thermometry[2] has been used to measure ΔT. Understanding these nonlinearities is important for the development of thermoelectric materials that aim to exploit quantum phenomena. 1. J.M. Wang et al, Nonlinear thermoelectric transport through a double barrier structure, Mod. Phys. Lett. B, 20, 215-223 (2006). 2. Hoffmann, E.A. et all, Quantum-dot thermometry, Appl. Phys. Lett. 91(25), 252114 (2007)

1Supported by the Office of Naval Research

C1.00107 Thermopower measurements of arrays of trigonal bismuth nanowires: the density, mobility, and charge-sign of Bi surface carriers. TITO HUBER, AJIBOLA ADEYEYE, TOSIN ODUNFA, Howard University, ALLA NIKOLAeva, LEONID KONOPKO, Academy of Sciences. Moldova, RYAN JOHNSON, MICHAEL GRAF, Physics Department. Boston College — We investigated the thermopower S of Bi nanowires with 20 nm < diameter < 200 nm) between 4 K and room temperature in well-characterized samples. Shubnikov-de Haas oscillations give evidence of light-effective-mass bulklike carriers, Dirac electrons and holes, and also high-effective-mass surface carriers. The latter are likely related to the surface states that are observed using ARPES of Bi surfaces (Hofmann, Prog. Surf. Sci. 81, 191 (2006)). Whereas the bulklike carrier’s concentration decreases for decreasing diameter in accordance with theoretical predictions (Lin, Sun, and Dresselhaus, Phys. Rev. 62, 4610 (2000)) for the quantum-confinement-driven semimetal-to-semiconductor transition, the surface carrier concentration is relatively independent of diameter. S exhibits a trend from positive towards negative values as the diameter decreases from 200 nm to 35 nm. The measurements are interpreted in terms of the diffusion thermopower model. We find that the S of the semiconductor nanowires is dominated by surface electrons.

1National Science Foundation. DMR. PREM Program.
C.100108 Thermoelectric Figure-of-Merit of Nanostructured Silicon with a Low Concentration of Germanium


We acknowledge funding support from UNLV presidential research award.

C.100109 Thermoelectric and electronic properties of AgSbSe$_2$

M. Kaur, Department of Electrical Engineering, University of Nevada Las Vegas, Ravish Kumar et al., J. Alloys Compds., 285 (1999) 48

We acknowledge funding support from UNLV presidential research award.

C.100110 Thermoelectric properties of mechanically milled AgSbTe$_2$

S. Veeramalai, Ravish Kumar, Department of Physics and Astronomy and HiPSEC, University of Nevada Las Vegas, Seigi Yoneda, Department of Physics and HiPSEC, University of Nevada Las Vegas — Cubic I-II-VI semiconductors have been studied widely for potential thermoelectric applications by several groups [1]. Recent investigations show minimal thermal conductivity for AgSbSe$_2$ and AgSbTe$_2$ resulting from intrinsic phonon scattering process due to strong anharmonicity in bonding [2]. AgSbSe$_2$ is structurally similar to chalcogenides and crystallizes in the cubic structure at ambient conditions [3]. The thermoelectric figure of merit, Seebeck coefficient and thermal conductivity were measured as a function of temperature from 10 K to 350 K. We have also measured the conductivity type, Hall coefficient and carrier concentration at ambient conditions. We compare our results with the ternary analogues. [1]. C. Wood et al., Prog. Phys. 51 (1988) 459 [2]. D. T. Morielli et al., Phys.Rev.Lett., 101 (2008) 035901 [3]. Ravish S. Kumar et al., J. Alloys and Compds., 285 (1999) 48

3We acknowledge funding support from UNLV presidential research award.

C.100111 Enhanced Thermoelectric Figure-of-Merit in p-type Nanostructured Bismuth Antimony Tellurium Alloys Made from Elemental Chunks

Yi Ma, Boston College, Qiang Hao, MIT, Bed Poude, Boston College, GMZ Energy, Inc., Yucheng Lan, Bo Yu, Dezhzi Wang, Boston College, Gang Chen, MIT, ZhiFeng Ren, Boston College, BOSTON COLLEGE TEAM, GMZ ENERGY, INC. COLLABORATION, MIT COLLABORATION — In this study, we use the ball milling and hot press technique to make nanostructured bulk bismuth antimony telluride from elemental chunks of bismuth, antimony, and tellurium. We show that a peak ZT of about 1.3 in the temperature range of 75 and 100 °C has been achieved. The ZT improvement is caused mostly by the lower thermal conductivity. Transmission electron microscopy observations of the microstructures suggest that the lower thermal conductivity is mainly due to the increased phonon scattering from the increased grain boundaries of the nanograins, precipitates, nanodots, and defects.

C.100112 Thermoelectric properties of Yb$_{14}$MnSb$_{11}$ from first-principles

J.-H. Song, Northwestern U., M. Kim, Ajou U., A.J. Freeman, Northwestern U. — The complex Zintl compound, Yb$_{14}$MnSb$_{11}$, has been recently given much attention as a high-performance thermoelectric due to its nearly twice the figure of merit (ZT) of p-type SiGe at high temperatures (> 900 K). Its high ZT can be attributed to low lattice thermal conductivity combined with a large Seebeck coefficient (S) and high electrical conductivity (σ) at high temperatures. To understand the thermoelectric properties of Yb$_{14}$MnSb$_{11}$ and to find possible improvements for thermoelectric performance, we have investigated its electronic structures and electrical transport properties (S,σ) using the highly precise FLAPW method with the local spin density approximation (LSDA) and LSDA+U methods. We have found significantly different spin moments of Mn between the LSDA and the LSDA+U methods. Also, we determined the anisotropy of the conductivity. The linear temperature behavior of the Seebeck coefficients will be discussed from and related to the electronic structures.

3Supported by NSF (through its MRSEC program at N.U.) and KRF (KRF-2008-313-C00218).

C.100113 Terahertz mixing in AlGaAs/GaAs 2DEG hot-electron microbolometers at liquid nitrogen temperatures

Kai Wang, Rahul Ramaswamy, Matthew Bell, Andrei Sergeev, Alesandr Verevkin, Gottfried Strauss, Vladimir Mitin, University at Buffalo, Darold Wobschall, Eensors Inc. — We investigate THz mixing based on electron heating of two-dimensional electron gas (2DEG) in semiconductor microbolometers. The 2DEG microbolometers were fabricated from AlGaAs/GaAs heterostructures and have dimensions of 3-20 µm between the Ohmic contacts and 50 µm in width. Significant efforts were made to get low Ohmic contact resistance for effective coupling to the THz antenna and to the intermediate frequency amplifier. We investigate mixing at sub-THz and THz frequencies. In the sub-THz range, a W-band Gunn diode operating at 82 GHz was used as a local oscillator. In the THz range we employ a Quantum Cascade Laser (QCL). The QCL is positioned in close proximity at different locations to optimize electromagnetic coupling. Experiments at sub-THz and THz frequencies give consistent data, which provide evidence that electron-heating is the major mechanism of mixing. Mixing experiments allow us to evaluate the mixer gain bandwidth and conversion loss. The results show that a heterodyne receiver, which combines AlGaAs/GaAs 2DEG hot-electron mixer with a QCL as the local oscillator, has great prospects for THz sensing with high spectral resolution and wide spectral bandwidth.

3This research was supported by NYSTAR and NSF SBIR
C1.00114 Design and operating regimes of quantum-dot photodetectors for room temperature operation

D. V. Anghel and D. Churochkin, Phys. Rev. B 78

Related publications:

in disordered crystals than in isotropic solids. We also point to the fact that the ratio of phonons and elastic waves in disordered crystals. In this model, the interaction strength depends on the orientation of the TLS with respect to the strain field

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The work is supported by AFOSR

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Russia — We apply the model introduced in Phys. Rev. B 78 to the wide absorption energy range of the visible light and the fast photo-induced charge injection from the dyes to the titania. The dyes are adsorbed on the Ti sites via the carboxyl group, but detailed adsorbed structures and effect on the electronic structures are unknown. We performed the first-principles calculations of the coumarin343 and NKX2311 dyes adsorbed on the rutile titania (110) for three types of the contact structures. We found that the bidentate type is energetically more stable than the ester-like and molecular types. The HOMO-LUMO gap of the NKX2311 is smaller than that of the coumarin343, consistent with the experiments. This work was partly supported by the RISS project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

The work is supported by NSF of R.O.C. under grand No. NSC 96-2112-M-110-008-MY2

C1.00115 Polarization dynamics within the polarization-switching hysteresis loop of VCSELs

JIN-ING TSAI, WANG-CHUANG KUO, CHUAN-PI HSU, Department of Physics, National Sun Yat-sen University, DA-LONG CHENG, Department of Computer and Communication, SHU-TE University, TSU-CHIANG YEN, Department of Physics, National Sun Yat-sen University — In the L-I curve of some VCSELs, distinct polarization switchings (PS) with a hysteresis loop are observed. In this research, PS at the center of the hysteresis loop was conducted by a manipulation of the operation conditions, enabling the polarization dynamics within the loop to be investigated. Experimental results revealed that the temporal behaviors of PS were different at the two ends of the PS hysteresis loop. A set of rate equations based on a linear gain model was employed to understand the polarization dynamics involved. Simulations indicated that the polarization dynamics could be attributed to the variation of the polarization-resolved gains within the PS hysteresis loop. More investigated results will be presented in the report.

C1.00116 Negative index of photonic crystal infiltrated with functional materials

RYOTARO OZAKI, Alan G. MacDiarmid NanoTech Institute, The University of Texas at Dallas, HIROSHI MORITAKE, Department of Electrical and Electronic Engineering, National Defense Academy of Japan, KATSUMI YOSHINO, Shimane Institute for Industrial Technology, ANVAR ZAKHIDOV, Alan G. MacDiarmid NanoTech Institute, The University of Texas at Dallas — We study 2D or 3D photonic crystals infiltrated with functional materials such as liquid crystal, or a highly polarizable medium. Liquid crystal molecular orientations in photonic crystals strongly influence the light propagation. We reveal that the negative index of the photonic crystal depends on the liquid crystal molecules, which can be tuned by external electrical field or temperature. On the other hand, we also study negative index of photonic crystal with a highly polarizable medium having a frequency dependence of permittivity. Around anomalous dispersion frequency range, the photonic crystal with a highly polarizable medium shows unique characteristics due to coupling with polariton.

C1.00117 First-principles study of atomic and electronic structures of coumarin dyes adsorbed on titania surface

HIROYOSHI MOMIDA, Institute of Industrial Science, University of Tokyo, TAKAHISA OHNO, CMSC, National Institute for Materials Science and Institute of Industrial Science, University of Tokyo — The coumarin dyes are good photo-sensitizers for the dye-sensitized solar cell due to the wide absorption energy range of the visible light and the fast photo-induced charge injection from the dyes to the titania. The dyes are adsorbed on the Ti sites via the carboxyl group, but detailed adsorbed structures and effect on the electronic structures are unknown. We performed the first-principles calculations of the coumarin343 and NKX2311 dyes adsorbed on the rutile titania (110) for three types of the contact structures. We found that the bidentate type is energetically more stable than the ester-like and molecular types. The HOMO-LUMO gap of the NKX2311 is smaller than that of the coumarin343, consistent with the experiments. This work was partly supported by the RISS project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

C1.00118 ABSTRACT WITHDRAWN —

C1.00119 Coiled-Coil Helix-Bundle Peptide-Polymer Conjugates

JESSICA SHU, CEN TAN, YU-JA HUANG, Department of Materials Science and Engineering, University of California, Berkeley, TING XU, Department of Materials Science and Engineering, Department of Chemistry, University of California, Berkeley — Peptide-polymer conjugates have the potential to combine the advantages of synthetic polymers and peptides and may lead to hierarchically ordered, functional soft materials. Maintaining the structure and function of the peptides upon polymer conjugation is essential. Here, we present a solution study of three families of peptide-polymer conjugates to systematically investigate the effect of conjugated polymer on the peptide’s secondary and tertiary structures using a photoactive, heme-binding 4-helix bundle. In particular, we focused on the effect of the peptide-polymer conjugate’s architecture (side conjugation versus end conjugation) and the hydrophobicity of the synthetic polymer (polystyrene versus poly(ethylene glycol)). Upon attachment of polymer to the peptide N-terminus, the secondary structure was destabilized and the functionality within the bundle was inhibited. The effect was less dramatic with PEG conjugation in comparison to the hydrophobic PS. Upon attachment of PEG to the exterior of the coiled-coil helix bundle, the peptide secondary and tertiary structures were stabilized, and the functionality within the bundle was preserved.

C1.00120 COMPLEX STRUCTURED MATERIALS —

C1.00121 Anisotropic glasy properties—a theoretical model

DRAGOS-VICTOR ANGHEL, Department of Theoretical Physics, Horia Hulubei National Institute of Physics and Nuclear Engineering, DMITRIY CHUROCHKIN, R & D Institute “Volga” - Saratov 410052, Russia — We apply the model introduced in Phys. Rev. B 75, 064202 (2007), to calculate the anisotropy effects in the interaction of two level systems with phonons and elastic waves in disordered crystals. In this model, the interaction strength depends on the orientation of the TLS with respect to the strain field through a $6 \times 6$ symmetric tensor of deformation potential parameters, $|\mathbf{R}|$. The structure of $|\mathbf{R}|$ is similar to the structure of the tensor of elastic stiffness constants, in the sense that they are determined by the same symmetry transformations. In this way, we emphasize the anisotropy of the interaction of elastic waves with the ensemble of two-level systems in disordered crystals. We also point to the fact that the ratio $\gamma_1/\gamma_1$ has a much broader range of allowed values in disordered crystals than in isotropic solids.

Related publications:


1Work partially supported by the NATO grant, EAP.RIG 982080.
C1.00122 Brillouin light scattering measurements of high modulus glasses produced by physical vapor deposition. KENNETH L. KEARNS, Department of Chemistry, University of Wisconsin-Madison, TIM STILL, Max Planck Institute for Polymer Research, GEORGE FYTAS, Max Planck Institute for Polymer Research, Department of Chemistry, University of Wisconsin-Madison — Physical vapor deposition was used to create low enthalpy, high density glasses of indomethacin (IMC). Brillouin light scattering was employed to measure the longitudinal and transverse sound velocities of the stable vapor-deposited glass, supercooled liquid, and the ordinary glass formed from cooling the liquid. Both Young and shear high frequency moduli were approximately 20% greater for the vapor-deposited sample as compared to the ordinary glass. The isothermal transformation of the high modulus glass to the supercooled liquid was 10,000 times slower than the structural relaxation time of the supercooled liquid at T = 10 K. Additionally, the spectrum for both phonon polarizations broadens during the isothermal transformation, which suggests that the stable vapor-deposited glass and supercooled liquid coexist for long periods of time at a single temperature.

C1.00123 Kinetics of Gold Nanoparticle Formation1, ASHLEY CETNAR, Grove City College, SREERAM CINGARAPU, KENNETH KLABUNDE, Kansas State University — My objective was to understand the chemical details of an important method of producing monodisperse nanoparticles. The nanoparticles synthesized are gold ligated by thiol ligands. The nanoparticles average 5 nanometers in diameter with about 5000 gold atoms and 600 thiol ligands per particle. The two methods used to prepare the particles are the solvated metal atom dispersion method and the inverse micelle method. Both processes break the gold into nanoparticles and are ligated to protect the particles from aggregation. After the nanoparticles are produced they are made monodisperse by digestive ripening. Digestive ripening occurs when the polydispersed product is refluxed over time. During this illusive procedure the multi-sized particles all become uniform in size. During reflux, the samples are analyzed by UV spectroscopy. The spectroscopy reveals a plasmon emitted from the nanoparticles at 530 nm from a standard sample of 1:30 gold to ligand ratio. During the reflux procedure, the gold Plasmon peak narrows and the peak becomes steeper. Over time, the peak of the Plasmon seems to be red shifted. As the amount of ligand varied the gold plasmon appeared to shift.

1This research opportunity was made possible by the National Science Foundation REU program.

C1.00124 Atomistic Mechanism of Catalyzed Growth of Silicon Nanowire, SEUNGHWA RYU, Physics Department, Stanford University, WEI CAI, Mechanical Engineering Department, Stanford University — Understanding the growth mechanism of semiconductor nanowire (NW) from catalyzed droplet is important for better control of the growth speed of NWs by chemical vapor deposition (CVD) over silicon. We used the Vapor-Liquid-Solid (VLS) process. To accurately describe the interatomic interaction between gold and silicon atoms, we developed a Au-Si binary potential based on modified embedded-atoms method (MEAM), which is benchmarked against the experimental binary phase diagram and mixing enthalpy. Advanced sampling method is employed to obtain the critical island at the liquid(Si Au alloy) - solid(silicon nanowire) interface. The dependence of the nucleation rate of the critical island on temperature and Si supersaturation is compared with experimentally observed NW growth rate and conditions of growth anormally such as kinking.

C1.00125 Self-Assembly of CdSe and PbS/PbSe Quantum Dots on Gold and other Surfaces Using Dithiol Functionalization, JEFFREY SCHWARTZ, MIAOXIN ZHOU, ANVAR ZAKHIDOV, The University of Texas at Dallas — CdSe and PbS/PbSe quantum dots were deposited onto gold surfaces functionalized with self-assembled monolayers of dithiol molecules. Separately, quantum dots were treated in solution with dithiols to create linked quantum dot chains and then deposited onto gold and other surfaces. Analysis of the samples via atomic force microscopy and scanning tunneling microscopy was performed in order to characterize the samples and determine the ordering and level of coverage of the quantum dots on the substrate surface. We found that increasing the bulkiness of the dithiol ligands leads to increased electrical conductivity of self-assembled quantum dot layers and found the optimal conditions for maximum coverage and best ordering. This research is done with the intention of using linked, ordered, quantum dot chains in polymer solar cell devices, and embedding quantum dots inside opals and inverse opals to create negative index materials.

C1.00126 Energetic and structural analysis of 102-atom Pd-Pt nanoparticles1, RAFAEL PACHECO-CONTRERAS, DIFUS, ALVARO ARTEAGA-GUERRERO, DFUS, DORA JULIA BORBON-GONZALEZ, Dept de Matematicas, UNISON, ALVARO POSADA-AMARIILLAS, DIFUS, J. CHRISTIAN SCHLENION, Max Planck Institute for Solid State Research, ROY L. JOHNSTON, School of Chemistry, University of Birmingham — We present an extensive study of the structural and energetic changes of 102-atom Pd-Pt nanoparticles as a function of composition m, where the interatomic interactions are modeled with the many-body Gupta potential. The minimum energy structures are obtained through a genetic algorithm. The excess energy is calculated, as well as the pair distribution function g(r). The radial distribution of the atoms is computed for each composition; the result indicates a multi-layer segregation for some compositions, with a shell growth sequence as follows: a core with a small number of Pd atoms and the external shell consists of Pt atoms. A region where Pd and Pt atoms are mixed is observed between the outermost and intermediate shells. Furthermore, the pure Pd102 and Pt102 nanoparticles have the same structure, while a variety of different structures are observed for the bimetallic clusters.

1APA acknowledge CONACyT-Mexico for financial support through project 24060.

C1.00127 Electronic Structure Models of Phosphorus Delta-Doped Silicon, OLIVER WARSCHKOW, DAMIEN J. CARTER, Centre for Quantum Computer Technology, School of Physics, The University of Sydney, NIGEL A. MARKS, Nanochemistry Research Institute, Curtin University of Technology, DAVID R. MCKENZIE, Centre for Quantum Computer Technology, School of Physics, The University of Sydney — We report a full density functional theory treatment of phosphorus delta-doped silicon. A particular difficulty of this system is associated with the large delocalization lengths of donor electrons in the host. To this end, we use large asymmetric unit cells with up to 800 atoms, and we obtain first-principles doping potentials, band energies and donor electron distributions. We additionally examine the electronic effects of overlapping doping potentials when two delta-doped planes are bought into proximity.

C1.00128 Experimental and theoretical spectroscopic studies of dye modification in synthetic Maya Blue pigment1, LAYRA REZA, FELICIA MANDCIU, Physics Department, ALEJANDRA RAMIREZ, RUSSELL CHIANELLI, Materials Research and Technology Institute, University of Texas at El Paso, El Paso, Texas 79968 — Maya pigments are hybrid organic/inorganic materials with multiple technology applications that possess unprecedented stability with respect to harsh environment conditions. In this investigation, we address the question of how the organic indigo dye modifies as it binds to the inorganic palygorskite clay to form a pigment similar to Maya Blue after a heating treatment is applied. Both infrared and Raman spectroscopic data demonstrate the disappearance of nitrogen-hydrogen (N-H) bonding, as the indigo molecule incorporates into the inorganic palygorskite material. This effect suggests a transformation of the dye from indigo to dehydroindigo. Furthermore, the Raman and infrared absorption results demonstrate partial elimination of the selection rules for the centrosymmetric indigo, which provides further evidence for this conversion. Theoretical spectroscopic studies are also addressed in this investigation to confirm the transformation of the dye into dehydroindigo.

1This work was supported by NSF-MRI grant # 0723115.
C1.00129 Spectroscopic study of thioindigo-mineral composite1, WILLIAM DURRER, FELICIA MANCIU, Physics Department, ALEJANDRA RAMIREZ, Materials Research and Technology Institute, JAYESH GOVANI, Physics Department, RUSSELL CHIANELLI, Materials Research and Technology Institute, The University of Texas at El Paso, El Paso, Texas 79968 — We report in this study structural changes taking place for the thioindigo-clay mixture in forming a pigment similar to Maya Blue. Different proportions of dye concentrations relative to that of the mineral, as well as different heating times, were applied in pigment synthesis and the outcomes were investigated using FT-IR and FT-Raman spectroscopy. For the pigment samples, the FT-IR peaks at 1627 cm−1 are attributed to a downshifted C=O stretching mode of thioindigo due to dye-clay interaction. This interpretation is corroborated by FT-Raman C=O peaks with 14 cm−1 shifts to lower frequency for the pigment relative to thioindigo alone. Additional Raman scattering between 550 cm−1 and 650 cm−1 also suggests dye-clay interaction through metal-oxygen bonding. We thus consider the possibility of hydrogen bonding between silanol and carbonyl dominating at lower dye concentration, with mostly metal-oxygen bonding at higher dye concentration.

1This work was supported by NSF-MRI grant # 0723115 and the DOE (BES) “Gateway Program.”

C1.00130 Inverse magnetoelectric effects in a bilayer of ferrite and graded piezoelectric, VLADIMIR PETROV, Novgorod State University, GOPALAN SRINIVASAN, Oakland University — Magnetoelectric (ME) effects in a piezoelectric-magnetostrictive composite are mediated by mechanical stress. An applied electric field, for example, will result in piezoelectric strain in the composite and will lead to a shift in ferromagnetic resonance (FMR) in the ferrite. This work is on modeling of magnetoelectric interactions under FMR in a bilayer of ferrite and functionally graded piezoelectric. We show that an enhancement of the strength of ME interaction at FMR is possible with the use of piezoelectric coefficient-graded ferroelectric with the grading axis perpendicular to the sample plane. In this case, the thickness dependence of the piezoelectric coefficients leads to an additional bending strain, resulting in an increase in the FMR line shift. Expressions have been obtained for the electrically induced magnetic resonance line shift, taking into account the effect of grazing and substrate clamping. The obtained results are applied to the cases of single crystal yttrium iron garnet (YIG) and graded lead magnesium niobate-lead titanate (PMN-PT). A 40% increase in the shift of FMR line is predicted for graded systems compared to homogeneous piezoelectric composition.

C1.00131 Microwave Magnetoelectric Interactions in Ferrite-Piezoelectric Bilayers1, ALEXANDER TATARENKO, Oakland University, VIKAS MATHE, Pune University, GOPALAN SRINIVASAN — The measurement of the strength of microwave magnetoelectric (ME) interactions through ferromagnetic resonance (FMR) in bilayers of single crystal ferrite-piezoelectric oxides is reported. An electric field E produces a mechanical deformation in the piezoelectric phase, resulting in a shift in the resonance frequency for the ferrite. The strength of ME coupling is obtained from data on frequency shift vs E. Studies were performed on bilayers with single crystal yttrium iron garnet (YIG) films or single crystal nickel zinc ferrite and single crystal lead zirconium niobate-lead titanate (PZN-PT) or polycrystalline lead zirconate titanate (PZT). The samples were positioned in a microstrip-line-alumina ground plane structure. Resonance profiles were with a vector network analyzer obtained for E = 0-8 kV/cm for in-plane magnetic fields H. Important results are as follows. (i) The ME coupling in the bilayers is stronger in bilayers with PZT than for PZN-PT. (ii) The coupling is a factor of 2 stronger in samples with nickel zinc ferrite than for YIG. The bilayers are potentially useful for E-tunable microwave resonators, filters and phase shifters.

1Supported by grants from ARO and ONR.

C1.00132 Magnetic field gradient induced magnetoelectric response of piezoelectric-magnetostrictive laminates1, GOPALAN SRINIVASAN, Oakland University, VLADIMIR PETROV, Novgorod State University — Magnetoelectric (ME) effects in a piezoelectric-magnetostrictive composite are mediated by mechanical stress. The ME coupling in composites when subjected to a bias magnetic field and an ac magnetic field leads to an induced voltage that is directly proportional to the applied ac magnetic field amplitude. We discuss here the theory of ME interactions in a piezoelectric-magnetostrictive laminate which is subjected to a non-uniform bias magnetic field. The model predicts that the induced ME voltage will include an additional term which is proportional to the field gradient provided that the gradient direction is perpendicular to the laminate plane. The supplementary term in the ME voltage can be attributed to flexural deformations due to stress irregularity in the magnetostrictive component. As an example, the gradient magnetic field induced ME effect is considered for a bilayer of Terfenol-D and lead zirconate titanate. The ME voltage coefficient at electromechanical resonance is expected to exceed the low-frequency value by two orders of magnitude.

Supported by the National Science Foundation and the Russian Foundation for Basic Research.

C1.00133 Controlling the percolation behavior of conductor-insulator composites by changing the granular size of insulators1, KAZUHITO SHIDA, RYOJI SAHARA, HIROSHI MIJUSEKI, YOSHIYUKI KAWAOZOE — The critical behavior of percolation model does not depend on the detail of the embedding lattice. This fact can be a hard obstacle when one attempt to modulate and control the characteristics of the composite materials because the limit of modulation is limited by the percolation threshold, as in the case of substitution of expensive conductor materials by inexpensive insulator materials. Many attempts to solve this problem by changing the sizes and aspect ratios of conductor particles, expecting their effect in enhancing conduction as a “bridge” is not working well. We report our attempt to realize the same goal by introducing size differences in the insulator particles, not conductor particles. The effective transition point observed is actually lowered to 0.52 by this modulation from about 0.59 of conventional site percolation model (2D). The statistical nature of this novel model, in particular the optimum design of insulator particle size distribution, is a completely new and interesting theoretical problem. Moreover, this is considered to be a promising technique to reduce the amount of expensive conductor, for example the Indium in typical transparent conductor film.

Supported by Ministry of Economy, Trade and Industry (METI).

C1.00134 Medium-range Order in Periodic Mesoporous Silica1, ELLA WAN, Ohio University, KUANGMIN LI, GANG CHEN, Ohio University — Periodic mesoporous materials contain ordered pores with diameters between 2 and 50 nm. In spite of their ordered pore structure, most periodic mesoporous materials do not possess crystalline pore walls, and the atomic origin of the uncrystallizable pore walls has been elusive. It is believed that the medium-range structure in such materials holds the key to the answer. To understand the medium-range order in periodic mesoporous materials, we select periodic mesoporous silica as a model system for this study. SBA-15 of various pore sizes (5-15 nm) have been synthesized through a self-assembly process using triblock copolymers as the structure-directing agents. X-ray scattering was used to characterize the materials. Pore widths and pore thicknesses of SBA-15 were measured by small-angle x-ray scattering, and the medium-range structure was characterized by wide-angle x-ray scattering. Effects of periodic pore structure and temperature on the medium-range order of amorphous pore walls have been identified. Our study provides atomic insights into the origin of uncrystallizable pore walls of periodic mesoporous materials in general.

1G. Chen acknowledges Ohio University start-up fund for supporting this work.
\( \lambda \) is the interaction parameter of the Luttinger liquid in an individual nanotube. We calculate the tunnel density of states, for two metallic carbon nanotubes. We demonstrate that for a small angle of crossing, \( \nu \) in them into 0D fullerenes. Unlike the well-known superatom states of 1D nanotubes, also study the superatom states of 1D - 3D solids, their cage size, and exo and endohedral doping by metal atoms. We by lowering the energy of superatom states from 3.5 eV, for single chemisorbed C\(_{60}\) molecules, by DFT calculations we investigate their origin and the factors that influence their energy and wave function hybridization into nearly-free electron bands in molecular solids. We show that the superatom states are derived from the universal image potential states of molecular sheets by rolling and wrapping them into 0D fullerenes. Unlike the well-known \( \pi \) orbitals, superatom orbitals hybridize more extensively among the neighboring molecules to form bands with nearly free-electron dispersion. The prospect of exploiting the strong intermolecular coupling to achieve metal-like conduction in applications may be attained by lowering the energy of superatom states from 3.5 eV, for single chemisorbed C\(_{60}\) molecules, to proximity of the Fermi level; therefore, we study how the superatom state energies depend on factors such as the aggregation into 1D - 3D solids, their cage size, and exo and endohedral doping by metal atoms. We also study the superatom states of 1D nanotubes. 

1. Min Feng, Jin Zhao, Hrvoje Petek

2. Motivated by the discovery of the superatom states of C\(_{60}\) molecules, by DFT calculations we investigate their origin and the factors that influence their energy and wave function hybridization into nearly-free electron bands in molecular solids. We show that the superatom states are derived from the universal image potential states of molecular sheets by rolling and wrapping them into 0D fullerenes. Unlike the well-known \( \pi \) orbitals, superatom orbitals hybridize more extensively among the neighboring molecules to form bands with nearly free-electron dispersion. The prospect of exploiting the strong intermolecular coupling to achieve metal-like conduction in applications may be attained by lowering the energy of superatom states from 3.5 eV, for single chemisorbed C\(_{60}\) molecules, to proximity of the Fermi level; therefore, we study how the superatom state energies depend on factors such as the aggregation into 1D - 3D solids, their cage size, and exo and endohedral doping by metal atoms. We also study the superatom states of 1D nanotubes. 

1. This research was sponsored by the Keck Foundation and DOE.

C1.00135 Fullerene-Polyhedral Oligosilsesquioxane Organic-Inorganic Hybrids and Applications as a Nanolayered Supercapacitor, YINGFENG TU, CHUN YE, WENBIN ZHANG, CHI-CHUN TSAI, BIN SUN, XIAOHONG LI, STEPHEN Z. D. CHENG — Fullerene and polyhedral oligomeric silsesquioxane (“POSS”) organic-inorganic hybrid material was synthesized by esterification of methano[60]fullerene carbocyclic acid (MFCA) with POSS-OH. The chemical structure was characterized and proven by matrix assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS), nuclear magnetic resonance (NMR), thermogravimetric analysis (TGA), SEC and UV-Vis spectroscopy. The material has high solubility (more than 10\( \% \)) in solvents like toluene, THF, chloroform and hexane. The material has high thermal stability: only 1\( \% \) of total mass lost at 350 \( ^\circ \) C and 50\( \% \) at 800 \( ^\circ \) C. At high concentrations, the solution of fullerene-POSS can absorb nearly the full spectra of the UV-Vis region (200 nm-700 nm). Crystals can be grown from chloroform solution, and the crystal structure was determined by transmission electron microscopy (TEM) and \( \pi \)-ray diffraction as an orthorhombic structure with \( a = 2.10 \text{ nm}, b = 1.06 \text{ nm} \) and \( c = 3.71 \text{ nm} \). This indicates a bilayer structure. The alternating layered structure of fullerene (conductive) and POSS (insulating) in the crystal can be used for applications such as supercapacitors.

C1.00136 Electronic properties of a coupled polyyacetylene chain, RAIMUNDO COSTA, University of Western Ontario, CELIO MUNIZ, Universidad Estadual do Ceara — We study a coupled polyyacetylene chain using a theoretical field formalism and verify that this structure presents a gap in its band structure. This energy gap is calculated in terms of a quantized effective mass that depends on the coupling between the polyyacetylene chains. As the coupling decreases the gap vanishes and we can restore the previous results of one single polyyacetylene chain. We show that there is a chiral broken symmetry. Electrons propagating in one direction are more energetic than electrons propagating in the other direction of the chain. A formalism is developed to show that there is a particle oscillation phenomenon analogous to Bloch oscillations. The conductivity of the system is also calculated.

C1.00137 Energy level curvatures, parametric motion of electron spectra in carbon nanotubes, ISA ZHAREKESHEV — We examine scaling properties of statistical spectral measures of single-walled nanotubes in the frame of a standard tight-binding model for modified quasi one-dimensional disordered systems. Numerical-scaling analysis is performed for the energy correlation function, the spectral factor and the distributions of the level curvatures and velocities. Non-analyticity at the zero velocities and curvatures is found, which can be lifted by applying a moderate magnetic field. In the limit of weak disorder and at B=0 the level curvature distribution does not entirely obey Wigner-Dyson statistics, but is rather a non-trivial combination of the GOEs distributions depending of the aspect ration of the modelled nanotube. At strong disorder the curvature distribution deviates from the conventional log-normal statistics. The results are verified on the double-wall carbon nanotubes. Similar applications for graphene structures are considered.

C1.00138 The nearly free electron like superatom states in fullerenes and nanotubes, JIN ZHAO, MIN FENG, HRVOJE PETEK, Department of Physics & Astronomy, University of Pittsburgh — Motivated by the discovery of the superatom states of C\(_{60}\) molecules, by DFT calculations we investigate their origin and the factors that influence their energy and wave function hybridization into nearly-free electron bands in molecular solids. We show that the superatom states are derived from the universal image potential states of molecular sheets by rolling and wrapping them into 0D fullerenes. Unlike the well-known \( \pi \) orbitals, superatom orbitals hybridize more extensively among the neighboring molecules to form bands with nearly free-electron dispersion. The prospect of exploiting the strong intermolecular coupling to achieve metal-like conduction in applications may be attained by lowering the energy of superatom states from 3.5 eV, for single chemisorbed C\(_{60}\) molecules, to proximity of the Fermi level; therefore, we study how the superatom state energies depend on factors such as the aggregation into 1D - 3D solids, their cage size, and exo and endohedral doping by metal atoms. We also study the superatom states of 1D nanotubes.

1. This research was sponsored by the Keck Foundation and DOE.

C1.00139 Effect of Helical Perturbation on Exciton Binding Energy in Semiconducting Carbon Nanotubes, BENJAMIN TAYO, SLAVA ROTKIN, Dept. of Phys., Lehigh University — Exciton binding energy in the presence of an external DNA-induced helical potential is studied. Exciton energies are obtained by solving the Bethe-Salpeter equation within the tight-binding approximation. The quasi-particle wavefunctions and energies which enter the Bethe-Salpeter equation are “dressed” by the one-electron helical potential. This external potential, produced by helical DNA-wrapping, is modelled by applying a perturbation operator of the Coulomb interaction which breaks both translational and rotational symmetry. This lowering of symmetry induced by DNA-wrapping has far-reaching effects: the DNA changes the band gap of the nanotube thus modulating its electronic and optical properties. For instance, the helical perturbation uplifts the degeneracy on the angular momentum quantum number \( \lambda \), the interaction parameter of the Luttinger liquid in an individual nanotube. We calculate the tunnel density of states, \( \nu(\omega, x) \), as a function of energy, \( \omega \), and distance, \( x \), from the intersection. In contrast to a single nanotube, we find that, in the geometry of crossed nanotubes, conventional “rapid” oscillations in \( \nu(\omega, x) \) due to the plasmon scattering acquire an aperiodic “slow-breathing” envelope which has \( \lambda/\theta \) nodes.

2. This research was sponsored by the Petroleum Research Fund, DOE and Research Corporation.

C1.00140 Intersection of two nanotubes: density of states modulated by plasmon beatings with period governed by Luttinger-liquid parameter, VAGHARSH MKHITARYAN, YUAN FANG, JORDAN GERTON, EUGENE MISHCHENKO, MIKHAIL RAIKH, Department of Physics, University of Utah — We study theoretically the plasmon scattering at the intersection of two metallic carbon nanotubes. We demonstrate that for a small angle of crossing, \( \theta \ll 1 \), the transmission coefficient is an oscillatory function of \( \lambda/\theta \), where \( \lambda \) is the interaction parameter of the Luttinger liquid in an individual nanotube. We calculate the tunnel density of states, \( \nu(\omega, x) \), as a function of energy, \( \omega \), and distance, \( x \), from the intersection. In contrast to a single nanotube, we find that, in the geometry of crossed nanotubes, conventional “rapid” oscillations in \( \nu(\omega, x) \) due to the plasmon scattering acquire an aperiodic “slow-breathing” envelope which has \( \lambda/\theta \) nodes.

1. Supported by the Petroleum Research Fund, DOE and Research Corporation.

C1.00141 First principles study of energetic interaction of a carbon chain inside carbon nanotubes, LUIS AGUILERA, CINVESTAV, ALEJANDRO TAPIA, UADY, ROMEO DE COSS, CINVESTAV, CINVESTAV-UADY TEAM, MATERIAL SIMULATION TEAM — Recently has been reported a new type of one-dimensional carbon nanostructure. Carbon nanowires formed by a linear carbon-atom chain inside a carbon-nanotube have been observed using high-resolution transmission electron microscopy (HRTEM). In the present work, we have studied the energetic interaction and atomic forces inside of the (5,5) and (8,0) carbon nanowires, using the Density Functional Theory. The calculations were performed by the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. Analyzing the energetic interaction inside the carbon nanowires, we found that the linear carbon chain obtains a preferential position inside of the carbon nanowires.

1. This research was supported by the Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grants No: 82497 and 49985-J.
C1.00142 Physiosorption of Nucleobases on C(9,1) and C(6,5) Single-Wall Carbon Nanotubes: A Density Functional Theory Study, BRAHIM AKDIM, RUTH PACTHER, Wright Patterson Air Force Base, OH — Selective enrichment of single-wall carbon nanotubes (SWCNTs) of a specific chirality by single-stranded DNA sequences has been shown experimentally by Zheng et al. [JACS 2007, 129, 6094], where a larger enrichment of C(6,5) as compared to C(9,1), which are SWCNTs of the same diameter but different chirality, was demonstrated with alternating guanine and thymine (GT) bases. In this work, we report density functional (DFT) calculations of (G) and (T) nucleobase adsorption on C(6,5) and C(9,1) SWCNTs, in order to gain an understanding of the selective sorting, specifically regarding adsorption characteristics, interface energetics, and electronic structures, as dependent on the tube chirality, also including specifically an empirical dispersion correction in the DFT functional.

C1.00143 Novel One-Dimensional Organometallic Half Metals: Vanadium-Cyclopentadienyl, Vanadium-Cyclopentadienyl-Benzene, and Vanadium-Anthracene Wires, LU WANG, Physics Department, Peking University, ZIXING CAI, JUNYU WANG, JING LU, GUANGFU LUO, LIN LAI, JING ZHOU, RUIN GAO, DAPENG YU, GUANG-PING LI, WAI NING MEI, STEFANO SANVITO, PHYSICS DEPARTMENT, PEKING UNIVERSITY COLLABORATION, SICAS CENTER, LEE HALL, SUNY ONEONTA COLLABORATION, PHYSICS DEPARTMENT, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION, PHYSICS DEPARTMENT, TRINITY COLLEGE DUBLIN COLLABORATION — By using the density functional theory, we find that organometallic multidecker sandwich clusters Vn+1FeCp2n+1 (Cp = cyclopentadienyl), and V2nAntn+1 (Ant = anthracene) may have linear structures, and their total magnetic moments generally increase with the cluster size. The one-dimensional (VCp)n∞, (VBzVCp)n∞ (Bz = benzene), and (V2Ant)n∞ wires are predicted to be ferromagnetic half-metals, while the one-dimensional (VCpFeCp)n∞ wire is a ferromagnetic semiconductor. The spin transportation calculations indicate that the finite Vn+1FeCp2n+2 and Vn(FeCp2)n+1 sandwich clusters coupled to gold electrodes are nearly perfect spin-filters.

C1.00144 A Hybrid Density Functional Study Of Pure Ge And GeC Nanotubes: Zigzag Configuration, SOMILKUMAR J. RATHI, Colorado School of Mines, ASOK K. RAY, Department of Physics, The University of Texas, Arlington — Ab initio calculations within the framework of hybrid density functional theory and finite cluster approximation have been performed for the electronic and geometric structures of pure zigzag Ge and three different types of zigzag germanium carbide nanotubes from (3, 3) to (11, 11). Full geometry and spin optimizations with uncontracted symmetry have been performed. A detailed stability investigation of the topological classification of nanotubes with dependence of the electronic band gaps on the respective tube diameter, energy density of states, and dipole moments have been carried out for all the tubes. Using Mulliken charge analysis charge density distribution along the tube lengths is calculated. In depth structural analysis of the structure and molecular orbitals are also reported. From our results it is clear that type I zigzag nanotubes are the most stable structures. For pure Ge, type II, and type III GeC nanotubes the chemical bonding have mixed ionic-covalent character, while for type I GeC tubes are ionic in nature. A wide spectrum of band gap values is also obtained for these nanotubes. This present study also opens up the possibilities for numerous applications of hybrid Ge based nanotubes.

C1.00145 Deposition of Carbon Nanotube Networks for Electronics Applications, GARRETT WADSWORTH, TETYANA IGNAUTOVA, SLAVA ROTKIN, Lehigh University — The development of a simple though reliable deposition technique for Carbon Nanotube Networks on substrates would advance the production of working Carbon Nanotube (CNT) field effect transistors and other electronic devices immesurably. Our investigation of different methods and processes which would be able to reliably create conductive networks of CNTs was in the effort to achieve this goal. Samples were prepared using different stabilizing solutions such as aqueous Sodium Cholate and Dichloromethane along with several processes of physical application to create a network on various substrates. Characterization using several instruments, including a Keithley Semiconductor Characterization Station for transport measurements, SEM, and AFM was performed to gauge their conductivity and the relation to the sample morphology. The most consistent deposition of CNTs on SiO2/Si, SiN/Si and glass substrates occurs when using aqueous Sodium Cholate as the stabilizing solution, etching using a strong acid and rinsing to remove Cholate crystals.

C1.00146 Solution processed large area field effect transistors from dielectrophoretically aligned arrays of single-walled carbon nanotubes, ELIOT SILBAR, PAUL STOKES, YASHIRA M. ZAYAS-GONZALEZ, SAIFUL I. KHONDAKER, University of Central Florida, Nanoscience Technology Center and Department of Physics — Solution processed electronic devices have attracted tremendous attention because of their ease of processability, low cost of fabrication, and their ability to cover large areas. Over the last few decades, a tremendous amount of effort has been dedicated to improve device performance of solution processed organic field effect transistors (FETs). However, despite all these efforts, typical field effect mobilities for these devices are usually on the order of ∼ 0.1 cm²/Vs, and can vary rarely reach ∼ 1.0 cm²/Vs. We demonstrate solution processable large area field effect transistors (FETs) from aligned single-walled carbon nanotubes (SWNTs) arrays. Commercially available, surfactant free SWNTs suspended in aqueous solution were aligned between source and drain electrodes using AC dielectrophoresis. After removing the metallic nanotubes using electrical breakdown, the devices displayed on-off ratios up to 10⁸. The devices showed p-type FET behavior with maximum field effect mobility of 27.1 cm²/Vs, two orders of magnitude higher than solution processed organic FET devices.

C1.00147 Energy transfer between Rear Earth ions and Carbon Nanotubes, TETYANA IGNAUTOVA, HIKMAT NAJAFOV, SLAVA V. ROTKIN, Lehigh University, Physics Department, 16 Memorial Drive East, Bethlehem, PA 18015 — We investigate a potentiality of rare earth (RE) ions for the sensibilization of the carbon nanotubes (NT) luminescence via the resonance-type energy transfer expected from the appreciable spectral overlap. In this study we mainly focus on the time-resolved spectroscopy of selectively excited Tb³⁺ and Eu³⁺+ ions in water solution containing a high concentration of DNA-wrapped NT showed a clear sign of transfer from RE to NT. We propose that the electrostatic attraction between negatively charged DNA phosphate groups and positively charged RE ions (Tb³⁺ and Eu³⁺) in water solution resulted in RE-DNA-NT complex formation with a suitable inter-species spacing for the energy transfer from RE to NT as well as the appreciable spectral overlap. The transfer has been confirmed by small (<10%) but systematic shortening of the RE emission in water solution containing DNA-wrapped NT.

C1.00148 Optoelectronic Characterization of Nafion-gated Nanotube FETs, HAPPINESS MUNEDZIMWE, Lehigh University, IBE Dept., 200 West Packer Ave, Bethlehem, PA 18015, SLAVA V. ROTKIN, Lehigh University, Physics Dept., 16 Memorial Dr. East, Bethlehem, PA 18015 — Optoelectronic probing is a routine way of characterizing standard semiconductor devices. For Carbon Nanotubes Field Effect Transistors (CNT FETs) made on silicon, however, it is a challenge to distinguish between intrinsic and ambient/substrate effects. Photo voltages at the Si-SiO2 interface often dominate the characterization. Back gated FETs systems also exhibit very high gating voltages. Iononic substrates allow higher gating efficiencies and at lower voltages. We report significant transconductance and photo modulation at gate voltages peaking around 5V with Nafion-117 ionomer as substrate which is ten times less than for typical Si systems. We use a generic back-gated FET geometry for characterizing gating performance and the trapping processes at the Nafion–CNT layer interface. Typical signal rise and decay times are of the orders 10 s and 100 s respectively, consistent with charge trapping inside the ionomic polymer. The close similarity between electrostatic gating and photo-gating signal profiles makes the latter a plausible explanation for photo-conductance characterization mechanism in our samples.
C1.00149 Catalytic behavior of Graphene/CNT composites in DSCs, JOSEF VELTEN, ANVAR ZAKHIDOV, University of Texas, at Dallas, DILLIP PANDA, LYNN DENNAY, ATtila MOZER, DAVID OFFICER, University of Wollongong — This presentation demonstrates the replacement of the Pt used in the counter electrode of a dye sensitized solar cell (DSC) by a nanocomposite of carbon nanotube with graphene layers. The I/V redox reaction of such DSC was studied using a composite of graphene flakes (obtained by reduction of graphene oxide) with either single wall or multiwall carbon nanotube sheets. This nanocomposite was deposited onto FTO coated glass and this electrode showed improved catalytic behavior beyond the use of carbon nanotubes alone for the charge transfer redox reaction. This paper also compares the use of the CNT/Gr composite counter electrode with the standard Pt counter electrode. The details of increased catalytic activity of Gr/CNT was studied by impedance spectroscopy and the origin of the enhanced electron transfer at the Gr interface is discussed in terms of local states at atomic edges.

C1.00150 Thermal Properties of Carbon Nanotube and Nanofiber Nanopapers: Finite Element Analysis, LAWRENZO D. MOSES, ALPER BULDUM, Department of Physics, The University of Akron — Carbon nanotube and nanofiber nanopapers are promising candidates as electronic thermal management materials. Here we present finite element method calculations of nanotube-nanotube, nanofiber-nanofiber junctions and extended two dimensional structures (nanopapers) containing these junctions. In the studies of individual junctions, different nanotube/nanofiber diameters, size of contact area and effects of fusing are considered. In the studies of nanopapers, different morphologies, effects of junction-junction separation are considered and thermal transport through multiple layers are studied.

1Supported by ODOD, Third frontier RCP.

C1.00151 Combined transport and Raman measurements on individual carbon nanotubes, MARKUS ALHLSKOG, OLLI HERRANEN, JYRI RINTALA, ANDREAS JOHANSSON, MIKA PETTERSSON — Combined techniques for measurement of structural, transport, and spectroscopic properties of individual carbon nanotubes are very important for current progress in the physics of these materials. We have measured the Raman spectra of individual single walled nanotubes that are electrically contacted with lithographically fabricated microelectrodes on Si/SiO2 substrates. The G-band of the Raman spectra have characteristic features for metallic and semiconducting tubes that we are able to discern. This conclusion is confirmed by transport measurements that unambiguously distinguish between the two types of tubes.

C1.00152 Contact Resistance, Electrical Breakdown and Temperature-Dependent Conductance of Multi-Walled Carbon Nanotubes, XIANGYU CHEN, Department of Physics, Stanford University, DEJJ AKINWANDE, H.-S. PHILIP WONG, Department of Electrical Engineering, Stanford University — Contact resistance has always been one of the major issues for applications of carbon nanotubes such as interconnects for VLSI chips, etc. In order to study the physics of contact between carbon nanotubes and metal, the temperature dependence of contact resistance between carbon nanotube and different metals (Cr/Au, Pd, Ti/Au, etc.) in an extended temperature range (4K to 400K) are explored. These data provide insight into the carrier transport between metal and carbon nanotubes. In addition, the temperature coefficient of the resistivity of multi-walled carbon nanotubes (MWCNT) of different lengths in the temperature range from 4K to 400K are measured and compared with theoretical calculations. By studying the temperature-dependent conductance, we are able to understand carrier transport in MWCNTs at low temperatures. The electrical breakdown behavior of MWCNT is also studied. Information from shell-by-shell breakdown provides insight about the critical current density and inter-shell conductance at different temperatures.

C1.00153 Quantized Conductance and Residual Resistance in Nanowires, CHARLES MILNER, WOO-JOONG KIM, STEVE LAMOREAUX, Yale University — Conductance in nanowires is quantized in units of $G_0 = \frac{2e^2}{h}$. Nanowires can be formed by momentary contact between the ends of macroscopic metallic wires. During the final stage of their rupture, the conductance of the wires drops in a stepwise fashion. However, these steps do not necessarily fall on integer multiples of $G_0$, because of a possible presence of residual resistance in the system. Using gold, we have observed the characteristic steps of quantized conductance. We have also found evidence of residual resistance. Looking forward, we plan to increase the precision of our conductance statistics by implementing automated data acquisition in order to explore the origin of residual resistance in different metallic wires, such as copper and silver. By examining the sample quantized conductance, we hope to find particular characteristics in metals which give rise to residual resistance. We hypothesize that surface potential is one such characteristic.

C1.00154 Electronic Transport Properties on CNT-Metal NanoWire Junctions, SUNGJONG WOO, Univ of Mass Lowell, YOUNG-KYUN KWON, Kyung Hee University, Univ of Mass Lowell — In the devices using carbon nanotube(CNT), the contact property between CNT and metal nodes such as contact resistance is very important. The nanofabrication technology has now begun to get the experimental control of the junction at nanoscale. Using Density Functional Theory (DFT), we have calculated stable junction structures numerically between CNT and metal nanowires(MNW) such as gold. With the stable structures we have found, the transport properties are calculated using non-equilibrium Green’s function method. Different junction structures and their stabilities will be presented. The $I$-$V$ characteristics depending on different junctions and CNT chiralities will also be discussed.

C1.00155 Electronic properties of multiwall carbon nanotubes studied by rotation driven by AC electric fields, D. L. FAN, FRANK Q. ZHU, ROBERT CAMMARATA, C. L. CHIEN, Johns Hopkins University, MATERIALS TEAM, PHYSICS TEAM — We have studied the electronic properties of multiwall carbon nanotubes (MWCNT) using the frequency dependent rotation driven by AC electric fields. The rotation angle, speed, and chirality of MWCNT can be precisely controlled by the strength and frequency of the AC electric field. From the rotation characteristics, the imaginary part of the Clausius-Mossotti factor, which depends on the material, the geometry, and the AC frequency, has been determined from 0.05 to 1MHz. This work demonstrates a non-contact and non-destructive method for assessing the properties of nanotubes and other nanoentities. The rotation of MWCNT can also be exploited in nanoelectromechanical system (NEMS) with MWCNT acting as the rotating elements.

C1.00156 Conductance and elastic modulus of a strained carbon nanotube, FERAS ALZUBI, University of Central Florida, RONALD COSBY, Ball State University — A first principles atomistic calculation of the electrical conductance for a strained, single-wall metallic carbon nanotube segment containing forty eight atoms and placed between copper electrodes is reported. Density functional theory and a non-equilibrium Green’s function technique, encoded in a commercial software package, are used to calculate the electronic structure and current-voltage characteristics for small strains. A monotonic decrease in conductance with strain is predicted. Using force-strain data, a modified Young’s modulus is computed for isolated, stretched nanotube segments containing up to 192 atoms. The computational methods, parameters, Poisson ratios, area selections, and results are described.
Particle motion perpendicular to the graphene layer is calculated as a function of the velocity of the charged particle.

New doped nanotubes could have new applications in composite materials or in applications such as gas sensing or molecular detection.

Carbon Nanotubes have high potential for new materials based on their unique electronic and mechanical properties. They have found use in several fields, including composite materials, electronic nano-devices, catalysis, and energy storage, among others. Doping of nanotubes by exohedral or endohedral methods has been found to substantially modify their electronic structure, as well as their chemical reactivity. In this work, we present a density functional theory study of the electronic and mechanical properties of phosphorus and phosphorus-nitrogen substitutionally doped carbon nanotubes. It is found that doping with these atoms create localized states which modifies electron transport properties. The effects on mechanical properties will also be presented.

The energy loss of a fast charged particle probe incident on a geometry, associated with Klein tunneling in the graphene films and Andreev reflections at graphene interfaces. Gates are also provided for Fermi-level adjustments in the standard “FET” format. Samples are created by e-beam lithography.

Measurements of the thermal conductivity of graphene utilized a technique where the excitation laser initiated a heat wave. The data extraction procedure assumed plane heat waves. Realistic graphene flakes have variations in their width, and the heat wave front may deviate from the plane wave depending on the geometry of the flake. We report a numerical study of heat propagation in graphene flakes of arbitrary geometry. The thermal conduction was simulated using the finite element method. It was found that both the shape of the flake and the temperature distribution in the hot spot affect the extracted values. At the same time, for the flakes with the relatively constant width and the hot spot of the size comparable to the flake width, the thermal conductivity obtained using the simple plane-wave approximation give close values to our simulations. 


Thermal conductivity of graphene flakes of arbitrary geometry was calculated as a function of the thermal conductivity of the substrates. The results are interpreted in terms of the RKKY interaction and the Anderson impurity model.

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C1.00165 Water adsorption on a titanium-graphene surface with high metal density. GERARDO J. VAZQUEZ, EDUARDO RANGEL, GREGORIO RUIZ-CHAVARRIA, FERNANDO MAGANA, Instituto de Fisica, Universidad Nacional Autonoma de Mexico — Density functional theory and molecular dynamics were used to study the adsorption of a water molecule on a graphene layer modified with titanium at high metal coverage, with the Ti atoms located above the centers of the carbon hexagons. Two stable configurations for the titanium-graphene sheet were considered. One with one titanium atom per eight carbon atoms and the other with one Ti atom per two C atoms. We found that the water molecule is adsorbed on both configurations, but it is dissociated in two different ways forming $H$, $O$ and $HO$ when the interaction is with the second configuration.

C1.00166 Possible nano-spintronics devices with graphene as electron wave guides. KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — Another application of graphene to semiconductor spintronics devices is proposed theoretically. We have designed possible methods for fabrication of nano-scale device structures utilizing graphene as electron wave guides. Important techniques should be 1) formation of strong covalent bonding between a part of substrate and graphene, 2) creation of nano-sized superstructure with sharp edges inducing the graphene edge states[1] by controlling interface between external electrodes and graphene, and 3) creation of nano-sized quantum structures based on the spinodal nano-decomposition. Several test simulations on the electronic states of proposed structures and theoretical estimation of functionality of graphene as an electron wave guide for semiconductor spintronics devices are presented. [1] M. Fujita, K. Wakabayashi, K. Nakada and K. Kusakabe, J. Phys. Soc. Jpn. 65, 1920 (1996).

C1.00167 Effect of metal contacts on photocurrents in graphene transistors. ROKSANA GOLIZADEH MOJARAD, Purdue University, FENGNIAN XIA, THOMAS MUELLER, MARCUS FREITAG, YU-MING LIN, PHAEDON AVOURIS, IBM Thomas J. Watson Research Centre — We present theoretical explanation of photocurrent in graphene and investigate the effect of contact induced states on in-plan electric field in graphene. Contact induced states are similar to the well-known metal induced gap states (MIGS) in metal-semiconductor Schottky junctions, which typically penetrate a few atomic lengths into the semiconductor, while the depth of penetration decreases with increasing band gap. However, in graphene we find that these states penetrate a much longer distance of the order of the width of the contacts.

C1.00168 Micro-Raman imaging spectroscopy of suspended graphene. J. R. SIMPSON, Towson University, Towson MD 21222, A. R. HIGHT WALKER, Physics Lab, National Institute of Standards and Technology, Gaithersburg, MD 20899 — The recent observation of ultrahigh mobility, $> 200,000 \mathrm{cm}^2 \mathrm{V}^{-1} \mathrm{s}^{-1}$, in suspended and annealed graphene underscores the importance of environmental effects on graphene electronic properties. We compare the Raman spectra of graphene and chemically modified graphite oxide both in contact with and suspended above substrate surfaces. Graphene samples were prepared using micromechanical cleavage and chemically modified graphite flakes on silicon substrates with a thin, $\approx$ 300 nm, silicon oxide coating. Reactive ion etching patterns the substrates with circular holes, approximately $3 - 7 \mu m$ in diameter, etched through the oxide layer. We present spatially-resolved Raman spectra obtained in a scanning, confocal microscope configuration using 632.8 nm and 514.5 nm laser excitation.


C1.00169 Intrinsic and extrinsic temperature dependences of Raman spectra of graphene. DANER ABDULA, TANER OZEL, KWANGU KANG, DAVID G. CAHILL, MOONSUB SHIM, University of Illinois Urbana-Champaign — Implementation of single-layer graphene (SLG) into next-generation electronics is of high interest due to unprecedented transport capabilities. Therefore, the importance of SLG doping and vibrational band structure is pronounced, both of which can be characterized with Raman spectroscopy. This work offers insights on the temperature dependent behavior of energy and linewidth of $E_{2G}$-band and $A_1$-2D-band Raman spectral features of intrinsic and air-exposed SLG. Mechanically exfoliated graphene in air exhibits a G-band linewidth that increases with temperature between 298K and 573K but shows an opposite trend after annealing under Ar. The opposing temperature dependences are considered within the context of Kohn anomaly induced phonon softening and broadening. The primary cause of the changes in $E_{2G}$-phonon energy and the electron-phonon coupling is attributed to ambient $O_2$ shifting the Fermi level away from the Dirac point. Our results emphasize the need to consider sample environment when investigating electronic and vibrational properties of graphene as well as when they are utilized, for example, in devices where SLG would undergo lithographic processing or even be operated in contact with various materials that may compromise its supposed high performance.

C1.00170 Conductance gaps modulation by periodic perturbations in graphene nanoribbons. M. PACHECO, L. ROSALES, Z. BARTICEVIC, U. Santa Maria, A. LEON, U. Diego Portales, A. LATGE, U. Federal Fluminense, P. ORELLANA, U. Catolica del Norte — Recently we have shown that the quantum conductance of a single molecule absorbed to the GNR shows the presence of Fano antiresonances at the energy levels of the molecule, suggesting that the GNR can be used as a spectrometer sensor [1]. When groups of molecules are attached, forming a periodic-like structure the conductance of the system presents forbidden minibands. Here we present a theoretical study of the electronic and transport properties of periodic perturbations on graphene nanoribbons. We study super-lattices formed by linear organic molecules side-attached at the ribbon edges and also by periodic structures of antidots in the GNR. The electronic properties of the systems are studied by using first principle calculations (LSDA), and tight binding Hamiltonian models. The quantum conductance is calculated in the Landauer formalism, with real-space renormalization techniques to obtain the Green functions. A series of well defined gaps on the conductance as a function of the Fermi energy are observed. This behavior depends on the period and topology of the perturbations and on the aspect ratio of the system. Conductance gap modulations can be obtained, suggesting new applications in graphene based nano-devices. [1] L. Rosales et al., Nanotechnology 19,0665402 (2008).

C1.00171 Spin Dependent Transport in Graphene Nano Ribbon Devices1, SATOFUMI SOUMA, MATSUTO OGAWA, Dept. of Electrical and Electronics Eng., Kobe Univ., TAKAHIRO YAMAMOTO, Dept. of Material Eng., Tokyo Univ., KAZUYUKI WATANABE, Dept. of Physics, Tokyo Univ. of Science — Graphene is now one of the promising materials for future nanoelectronics. Especially graphene nanoribbon is attracting great attention since it possesses finite bandgap opening depending on the ribbon width and the transport orientation with respect to the graphene lattice. Another interesting property seen in graphene nanoribbon is the appearance of the “edge-spin” polarization at the edges of the zigzag-edged graphene nanoribbon. Recently it has been shown that such edge- spin polarization can be electrically controlled to induce the half-metallic band structure in such structures, meaning the electronic controllability of the spin current in such material. Therefore, toward the realization of the graphene nanoribbon spintronics, it is now important to study the spin- dependent transport characteristics in realistic device structure based on zigzag graphene nanoribbon. Here we present our numerical study of spin transport in zigzag-edged graphene nanoribbon transistor structures [1] using spin-density functional tight-binding method. Special attention is paid to the influence of edge roughness and electrostatic doping on the spin polarization and the spin current. [1] S.Souma, M.Ogawa, T.Yamamoto, K.Watanabe, J.Comp. Electron. 7, 390 (2008).

1This work was supported by KAKENHI (18749006)
C1.00172 Influence of an electric-field on electronic properties of few-layer armchair graphene nanoribbons1, Y.-C. HUANG, Center for General Education, Kao Yuan University, H.-C. CHUNG, Dept. of Physics, Natl. Cheng Kung University — In the presence of an electric field, the low-energy electronic properties of AB-stacked few-layer armchair graphene nanoribbons (AGNRs) are studied by using the tight-binding model. They are strongly dependent on the geometric structures (the interlayer interactions, the ribbon width \( N_y \), and the ribbon number \( N_x \)) and the field strength. The interlayer interactions significantly affect density of states (DOS), energy gap \( (E_g) \), band structure, and free carriers. DOS exhibits many special structures, including plateau, discontinuities, and divergent peaks. The effective electric field modifies the energy dispersions, alters the subband spacing, changes the subband curvature, produces the new edge state, switches the band gap, and causes the metal- semiconductor (or semiconductor-metal) transitions. In gapless AGNR, electric fields not only lifts the degeneracy of subbands at \( E_F \) but also induces an energy gap. \( E_g \) is dependent on the ribbon width, and the field strength. The semiconductor-metal (or semiconductor-metal) transitions occur in AGNRs in the increase in electric fields. Due to electric fields, the above-mentioned effects are completely reflected in the features of DOS, such as the generation of special structures, the shift of peak position, the change in peak height, and the alternation of band gap. The predicted electronic properties could be examined by the experimental measurements on absorption spectra and transport properties.

1This work was supported by the Taiwan National Science Council (NSC 97-2112-M-244-001-MY2)

C1.00173 Low-energy Landau levels of AB-stacked zigzag graphene ribbons1, YUAN-CHENG HUANG, Center for General Education, Kao Yuan University — The low energy bands of AB-stacked zigzag graphene ribbons in the presence of a uniform perpendicular magnetic field are investigated by the Peierls coupling tight-binding model. They are dominated by the B-field strength, the interlayer interactions, and the ribbon width. Many dispersionless Landau levels and parabolic energy bands exist along \( k_x \) and \( k_y \) directions, respectively. The former are doubly degenerate, while state degeneracy is absent for the latter. The occupied valence bands are asymmetric to the unoccupied conduction bands about the Fermi level. Such features are directly reflected in density of states. DOS exhibits a lot of asymmetric prominent peaks because of 1D parabolic bands. The predicted magnetoelectronic properties could be examined by the experimental measurements on transport conductance and absorption spectra.

1This work was supported by the Taiwan National Science Council (NSC 97-2112-M-244-001-MY2)

C1.00174 Quasiparticles for quantum dot array in graphene and the associated Magnetoplasmons1, GODFREY GUMBS, Hunter College of CUNY, OLEG BERMAN, New York City College of Technology of CUNY, PEDRO ECHENIQUE, Donostia International Physics Center (DIPC) — We calculate the low-frequency magnetoplasmon excitation spectrum for a square array of quantum dots on a two-dimensional (2D) graphene layer. The confining potential is linear in the displacement from the center of the quantum dot. Consequently, the corresponding Klein-Gordon equation may be solved analytically for the single-particle eigenstates since they are given by a simple harmonic oscillator operator. The electron eigenstates in a magnetic field and confining potential are mapped onto a 2D plane of electron-hole pairs in an effective magnetic field without any confinement. The tight-binding model for the array of quantum dots leads to a wavefunction with inter-dot mixing of the single-particle eigenstates. For chosen confinement, magnetic field, wave vector and frequency, we plot the dispersion equation as a function of the period \( d \) of the lattice. We obtain those values of \( d \) which yield collective plasma excitations. For the allowed transitions between the valence and conduction bands in our calculations, we obtain plasmons when \( d < 100 \AA \).

C1.00175 Temperature Programmed Desorption Study of Graphene Oxide, NICHOLAS CLARK, DANIEL FIELD, SIMONA RIEMAN, CARL VENTRICE, Texas State University, INHWAN JUNG, DONGXING YANG, RICHARD PINER, RODNEY RUOFF, University of Texas — Graphene oxide is an electrical insulator that shows potential for use in nanoscale electronic devices. An understanding of the thermal stability of graphene oxide sheets is important since the electrical, chemical, and mechanical properties of graphene oxide will change as it is reduced at elevated temperatures. In this study, graphene oxide films were grown by deposition of an aqueous solution of graphene oxide onto oxygen plasma cleaned silicon nitride on silicon substrates. The thermal stability of these films was studied by temperature programmed desorption under ultra-high vacuum conditions up to 350 °C. The primary decomposition components of the films are \( \text{H}_2\text{O}, \text{CO}_2 \) and \( \text{CO} \). Desorption of these components starts at \( \sim 70 \) °C and is completed by \( \sim 150 \) °C. Coverage dependent measurements indicate that the desorption kinetics are second order. An activation energy of 162 meV for \( \text{CO}_2 \) desorption has been determined.

C1.00176 Structural and electronic characterization of epitaxial graphene on SiC (0001) using scanning tunneling microscopy/spectroscopy1, DAVID TORRANCE, NIKHIL SHARMA, PHILLIP FIRST, Georgia Institute of Technology — Epitaxial graphene exhibits high-quality crystallinity and is compatible with current industrial fabrication methods, which makes it a strong candidate for future electronic devices. One important and contested aspect of this material system is the interface region between graphene and SiC, and how this reconstruction alters the growth rate, structure, and electronic properties of graphene films. We have investigated epitaxial graphene on SiC (0001) in the very early stages of ultra-high vacuum growth using scanning tunneling microscopy/spectroscopy (STM/STS). Topographical maps of monolayer graphene islands formed in the initial stages of epitaxial growth will be presented along with STM measurements of these features and the surrounding interfacial reconstruction. We further discuss transitions between regions of different structure.

1Work supported by NSF

C1.00177 Real-Time Path Integral Study of Electron Transport in Molecular Wires: A Constant Current Formulation and the Importance of Dissipative Processes, ROBERTO LAMBERT, KE DONG, NANCY MAKRI, University of Illinois at Urbana-Champaign — We report the results of real-time path integral calculations to study electron transport in molecular-wire models. The molecular wire system is modeled by a multi-site one-electron tight-binding Hamiltonian connected to two metal electrodes and coupled to a bath mimicking the dissipative effects of molecular vibrations. In order to maintain a steady current flow, we introduce a simple recharging model in which electrons are injected from the donor electron as needed to replenish charge lost to the acceptor, maintaining a constant electron population within the wire. Using real-time path-integral techniques, we study the conductance of the molecular wire model as a function of wire length, with emphasis on the effects of its dependence on dissipation.
C1.00178 Synthesis and spectroscopic characterization of cadmium sulfide nanowires1. NARAYAN KUTHIRUMMAL, College of Charleston, JASON REPPERT, Clemson University, BRIAN DEIHL, College of Charleston, APPARAO RAO, Clemson University — Pulsed laser vaporization method has been used for preparing cadmium sulfide (CdS) nanowires of 50–100 nm in diameter. The morphology and crystallinity of as-prepared CdS nanowires are studied by means of X-ray diffraction, scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HRTEM). Excellent ordering of the lattice planes perpendicular to the [001] plane has been observed. Photoacoustic (PA), UV-Vis, Raman, and photoluminescence spectroscopy have been used to measure the optical properties. PA spectra yield a steeper absorption edge for as-prepared CdS nanowires when compared to the conventional optical absorption spectrum. The increased steepness might be attributed to the well-ordered structure and size distribution. The data shows that PA spectroscopy is an excellent technique to investigate opaque and highly light scattering samples. Raman data suggests increased exciton-LO phonon coupling in CdS nanowires. The appearance of a narrow photoluminescence peak at 491 nm (FWHM of 9 nm) and the absence of emission above 500 nm demonstrate the high quality of nanowires.

1Supported by NSF-NUE (EEC0631442).

C1.00179 Confocal Raman microscopy of one dimensional cadmium sulfide nanorods. SRIKANTH SINGAMENI, MANEESH GUPTA, RUSEN YANG, ZHONG WANG, VLADIMIR TSUKRUK, Georgia Institute of Technology, GIT/MSE TEAM — CdS nanorods with various shapes (vertically aligned nanorods, nanobells, nanohelices, nanorings) have been synthesized using both vapor phase and solution growth methods. In the simplest example of a nanobell, the fast growth direction can be either (21T0) or (01T0) or (0001). Here, we show that confocal Raman microscopy can be employed as a fast and nondestructive analytical technique to identify the crystal planes and reveal the relative orientation of the ZnO nanostucture. Various features of the Raman spectrum of ZnO nanostuctures (presence of the A1(LO) mode, width of the E2 mode) were found to be sensitive to relative orientation of the incident source laser and the crystal plane. Furthermore, owing to the optical anisotropy of ZnO, Raman scattering from the substrate is modulated (either enhanced or suppressed with respect to the background) depending on the polarization of the incident light with respect to orientation of the nanobell. The results presented here describe a novel method to nondestructively identify the growth, relative orientation, and the waveguiding properties of the ZnO nanostuctures.

C1.00180 Characterization of SiC nanowires obtained from carbon black powder. MONIKA WIELIGOR, T. W. ZERDA, Texas Christian University — SiC nanowires were obtained by a reaction between vapor silicon and carbon black powder in vacuum at 1200°C. Their structures and properties were studied using X-ray diffraction, high resolution transmission microscopy, HRTEM, and Raman scattering techniques. We show that diameter of sintered nanowires depends on carbon black grade and its history of thermal treatment. SiC nanowires of diameter as small as 10 nm were obtained from graphitized furnace carbon blacks. Chemical composition of nanowires was similar for all samples, but concentration of structural defects varied and depended on carbon black surface properties and surface morphology. Stacking faults and twins dislocations were observed in all specimens and characterized by HRTEM, X-ray diffraction, and Raman spectroscopy.

C1.00181 Parallel Tandems of Dye Sensitized Solar Cells with CNT Collector. JOSEF VELTEN, CHAOCHEN YUAN, ANVAR ZAKHIDOV, University of Texas, at Dallas — In this presentation, we demonstrate the fabrication of monolithic parallel tandem dye sensitized solar cells using a semitransparent layer of carbon nanotubes. Each DSC sub-cell has titania photoelectrode with two different dyes: N 719 and N 330, which absorb light in different parts of solar spectrum. This layer of carbon nanotubes laminated on highly porous polymeric Millipore filter acts as both the collector of charge carrier and as the catalyst of the I3−/I− redox reaction that completes the function of the cell, overall allowing easier fabrication for tandem solar cell devices, with a potential for creating flexible devices in the future. The parallel tandem shows the total photocurrent which is nearly the sum of two I3− currents of constituent cells, and total Voc, which is average of two Voc, while conventional in-series DSC tandems show the lowest Voc, and slightly increased I3−[1]. Thus the higher efficiency can be achieved in parallel DSC tandems, and we discuss the physical reasons for this effect. [1] Yanagida, et.al. J. of Photochemistry and Photobiology A: Chemistry Volume 164, Issues 1-3, 1 June 2004, Pages 33-39

C1.00182 Chaotic Electronic Transport in Nanocluster Wires. M.S. FAIRBANKS, Department of Physics, University of Oregon, T.P. MARTIN, School of Physics, University of New South Wales, Australia, C.A. MARLOW, B.C. SCANNELL, Department of Physics, University of Oregon, S.A. BROWN, Department of Physics and Astronomy, University of Canterbury, New Zealand, R.P. TAYLOR, Department of Physics, University of Oregon — Electronic circuits featuring nanoscale devices are highly topical due to their potential for exhibiting novel device functionality and fundamental solid-state physics. Currents based on nanoclusters are particularly appealing because they “self-assemble” [1]. Here we develop a theoretical transport model for nanowires formed from nanoclusters. The wire width varies along the wire’s length, creating an array of connected cavities. The wire walls reflect electron trajectories through material-induced chaotic scatterers within each cavity. We discuss how the chaotic properties can be engineered to increase the conductivity’s sensitivity to electric and magnetic fields for use as novel sensors. [1] For example, J. G. Partridge, et al., Microelectronic Engineering 83, 1460 (2006).

C1.00183 Unusual Conductance in Cumulene Molecular Wires. JARIYANEE PRASONGKIT, Condensed Matter Theory Group, Dept. of Physics and Materials Science, Uppsala University, Sweden, ANTON GRIGORIEV, CMT Group, Uppsala, GÖRAN WENDIN, Department of Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg, Sweden, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — We report current-voltage curves and conductance of cumulene molecular wire suspended between Au(111) surfaces via thiolate bonds with full self-consistent ab initio calculation under external bias. The conductance of cumulene wires shows oscillatory behavior depending on the number of carbon atoms. Among all conjugated oligomers, we find that odd-number cumulene wires yield the highest conductance and present ballistic-like transport behavior. The wire width varies along the wire’s length, creating an array of connected cavities. The wire walls reflect electron trajectories through material-induced chaotic scatterers within each cavity. We discuss how the chaotic properties can be engineered to increase the conductivity’s sensitivity to electric and magnetic fields for use as novel sensors. [1] For example, J. G. Partridge, et al., Microelectronic Engineering 83, 1460 (2006).

C1.00184 QUANTUM FLUIDS AND SOLIDS —

C1.00185 Critical temperature of extremely confined bosons. P. SALAS, Posgrado en Ciencia e Ingenieria de Materiales, UNAM, M. DE LLANO, Instituto de Investigaciones en Materiales, UNAM, M. FORTES, F.J. SEVILLA, M.A. SOLIS, Instituto de Fisica, UNAM — The critical BEC temperature Tc of an ideal boson gas inside a layer structure simulated by a Kronig-Penney-like trapping potential is found to decrease as the separation between planes decrease to the order of the thermal wavelength λT ≡ h/√2mκkB T0 of the free boson gas at its critical BEC temperature T0 [1], where m is the boson mass. However, when the plane separation is less than λT, Tc increases to nearly T0. This phenomenon could be present in cuprate superconductors and explain why their transition temperatures increases as a function of pressure. [1] P. Salas, M. Fortes, M. de Llano, F.J. Sevilla and M.A. Solis, “Thermodynamic properties of bosons among Kronig-Penney layers,” to be published. We acknowledge the partial support from grant PAPIIT IN1114708.

C1.00186 NANOTECHNOLOGY/BIONANOTECHNOLOGY —
C1.00187 Silicon nanowires under high pressure, YUEJIAN WANG, Los Alamos National Lab — Silicon nanowires (Si NWs), one-dimensional single crystalline, have recently drawn extensive attention, thanks to their robust applications in electrical and optical devices as well as in the strengthening of diamond/SiC superhard composites. Here, we conducted high-pressure synchrotron diffraction experiments in a diamond anvil cell to study phase transitions and compressibility of Si NWs. Our results revealed that the onset pressure for the Si-I to Si-II transformation in Si NWs is approximately 2.0 GPa lower than previously determined values for bulk Si, a trend that is consistent with the analysis of misfit in strain energy. The bulk modulus of Si-I NWs derived from the pressure-volume measurements is 123 GPa, which is comparable to that of Si-IV NWs but 25% larger than the reported values for bulk silicon. The reduced compressibility in Si NWs indicates that the unique wire-like structure in nanoscale plays vital roles in the elastic behavior of condensed matter.

C1.00188 Improved Synthesis of Aligned Carbon Nanotube Arrays for Optical Applications, TRILOCHAN PAUDEL, YANTAO GAO, YUCHENG LAN, GRÉG MACMOHAN, KRZYSZTOF KEMP, MICHAEL NAUGHTON, ZHIFENG REN, Boston College — Vertically aligned carbon nanotubes were grown on the high temperature glass (Aluminosilicate, Corning 1737) substrates with improved characteristics compared to previous attempts. The glass substrates were first coated with a buffer layer of either Chromium or Titanium, thick enough to facilitate CNT growth, but thin enough as to be largely transparent. On the top of the buffer layer, a monolayer of polystyrene spheres was deposited with close compaction, and then a Nickel catalyst film was evaporated. The polystyrene spheres were then removed to obtain honeycomb Ni patterns. On top of the Ni patterns, vertically aligned carbon nanotubes were grown by the direct current plasma enhanced chemical vapor deposition (dc PECVD). These aligned carbon nanotubes, which can range in height from 0.5 to 10 microns, and in diameter from 50 to 350 nm, can then be coated with various dielectrics to function as components in optical waveguides, including solar cells.

C1.00189 Enhancement of LED Backlight by Metallic Nanostructures1, Y.D. YAO, J.K. WU, Department of Materials Engineering, Tatung University, C.Y. HSU, S.Y. HSU, P.K. WEI, Research Center for Applied Science, Academia Sinica, D.H. WEI, Department of Mechanical Engineering, National Taipei University of Technology, M.D. CHOUP, C.N. MO, R & D Center, Chung Hwa Picture Tube, Ltd. — Metallic nanostructures with different size on ITO coated glass substrates have been fabricated by using metal thin film deposition, electron beam lithography, and nanosphere lithography techniques for studying the light guide in a display system. The increase of extraction efficiency is based on scattering light from the trapped photons. With Ag and Au nanostructures in peripheral area of emitting region on the ITO coated glass substrates, the external quantum efficiency of devices increases by roughly 14% and with a 100 nm-width and 450 nm-period metallic nanowire structures, the light extraction can enhance up to 40% from the glass substrate. We demonstrated that with a proper metallic nanostructure in the backlight system of a LED device, the extraction efficiency could be efficiently enhanced.

1 This research was supported by the National Science Council of Taiwan and Chung Hwa Picture Tube, Ltd.

C1.00190 Modified Electric Force Microscopy combined with Atomic Force Microscopy Electrostatic Nanolithography, SERGEI LYUKSYUTOV, The University of Akron — A hybrid method, combining electrostatic nanolithography with modified electric force microscopy was used to characterize and study surface electric charging of high molecular weight (850000 mw and 110000 mw) polymethyl methacrylate and polystyrene films. Experimental protocol to manipulate an atomic force microscope tip included 1) Displacement of the vibrating tip to the level when the vibration amplitude largely damped; 2) Tip retraction at the distance varied between 1 to 100 nm with positive or negative tip bias. A modified Electric force microscopy maps electric charge distribution and its sign on the sample surfaces. Stable surface deformation related to nanoscale mass transport was associated with electric breakdown and negative surface charging, while a temporary viscoelastic surface deformation followed by surface relaxation was due to positive surface charging.

C1.00191 A Novel Carbon Nanotube Network and Aptamer Based Biosensor, Y. AL-TITI, W.G. MATTHEWS, University of South Florida — A carbon nanotube network field effect transistor (CNTN-FET) based biosensor for the detection of Tenascin C will be presented. The device consists of CVD-grown CNTNs incorporated into FETs coupled with surface bound DNA aptamers. The aptamer conjugated FET provides highly selective and sensitive detection of protein concentrations. The sidewalls of the CNTs initially were functionalized with a short oligonucleotide which has the dual functions of blocking non-specific binding and serving as a tether for the addition of another DNA strand. Specific detection was accomplished through hybridization of an aptamer for Tenascin C to which the complementary strand of our blocking sequence was added to the 5’ end. IV curves and conductance versus time were collected, demonstrating detection of each of the two DNA strands and the protein Tenascin C. The protein produced an undetectable signal in the absence of the aptamer, even at higher concentrations. Confirmation of adsorption of the oligonucleotide, hybridization of the aptamer, and binding of Tenascin C were each confirmed through fluorescence microscopy. The resulting device is an important step toward low cost, label-free biosensors.

C1.00192 Detection of α-fetoprotein in human serum using carbon nanotube transistor, HYE-MI SO, DONG-WON PARK, KRICT, SEONG-KYU LEE, Eulji University School of Medicine, BEOM SOO KIM, Chungbuk National University, HYUNJU CHANG, JEONG-O LEE, KRICT — We have fabricated antibody-coated carbon nanotube field effect transistor (CNT-FET) sensor for the detection of α-fetoprotein (AFP), single chain glycoprotein of 70 kDa that is normally expressed in the fetal liver, in human serum. The AFP-specific antibodies were immobilized on CNT with linker molecule such as pyrenebutyric acid N-hydroxysuccinimide ester. To prevent nonspecific adsorption of antigen, we performed blocking procedure using bovine serum albumin (BSA). Antibody-antigen binding was determined by measuring electrical conductance change of FET and took an average of thershold voltage change before and after binding. Also we checked concentration-dependent conductance change in human serum using both p-type SWNT-FETs and n-type SWNT-FETs.

C1.00193 Wrapping of a single bacterium with Functionalized - Chemically Modified Graphene (FCMG) sheets via highly specific protein-cell wall interaction, NIHAR MOHANTY, VIKAS BERRY, Kansas State University — Graphene has recently generated a lot of interest due to its unique structural and electrical properties. It’s micro-scale area and sub-nano-scale thickness coupled with ballistic electronic transport at room temperature, low Johnston noise and low charge scattering, have made it a gold mine for novel applications. Since its discovery in 2004, there have been a plethora of studies on characterizing its unique physical, chemical and electrical properties of graphene as well as on integrating it with various physical/chemical systems to utilize these properties. But there have been limited or no studies on the integration of graphene with living microorganisms or mammalian cells. Here we describe the novel wrapping of a single live bacterium (Bacillus cereus) with a chemically modified graphene sheet functionalized with the protein Concanavalin-A (Con-A) via the highly specific Con-A - Teichoic acid interaction. We are investigating the structural and the electrical properties of these novel bacteria-FCMG ensembles. Further, we are also interested in characterizing this wrapping process in detail by studying the kinetics and the mechanism of action of bacterial-wrapping via 3D modelling. This is a first step towards the live-bio-nano-integration of graphene which would open up avenues for applications as diverse as bio-batteries using the Geobacter to recombinant enzyme compartmentalization.
Liquid crystalline materials. A new concept of smectic LC lithography technique. Grown in microchannels from a mixture of LC molecules and fluorescent particles, TFCDs of the smectic LCs form by semi-fluorinated smectic liquid crystals (LCs). Combining with controlled geometry, i.e. microchannel, our smectic LC system exhibits high density of materials for the creation of lithographic templates. Here we report that perfect ordered-arrays of toric focal conic domains (TFCDs) covering large areas can be realized.

Nanotechnology. To date, several distinct organic building blocks—including colloids, block copolymers and surfactants—have been examined as potential systems for the lithographic fabrication of carbon nanotubes. In the approach mode, the elastic modulus showed linear fit to yield stress and exponential fit to particle size of latex. The results are compared with non-linear elastic models that predict power law and exponential fits. The model uses microscopic statistical mechanical theory, which describes glassy dynamics based on a non-equilibrium free energy that incorporates local cage correlations and activated barrier-hopping processes.

Computer Simulation of a Magnetized Two-Dimensional System. We used AFM to study Cantilever mechanics and Atomic Force Microscopy study of TEHOS. We performed extensive computer simulations on a two-dimensional electron system in a perpendicular magnetic field. The calculations cover the various values of the coupling parameters. The effect due to magnetic field is systematically studied as a function of coupling parameters for both static and dynamical properties.
C1.00203 Miscibility behavior of blends of spiropyran chromophore and mesogenic diacrylate1, HARRIS LAM, University of New Orleans, NAMIL KIM, THEIN KYU, University of Akron — The phase diagram of blends of photochromic molecule (spiropyran) and mesogenic diacrylate monomer (RM257) has been constructed experimentally and theoretically. The phase diagram involving solid-liquid phase transition has been investigated using differential scanning calorimetry (DSC) and subsequently the theoretical calculation was performed by self-consistently solving the combined free energies of Flory-Huggins (FH), Maier-Saupe (MS), and phase field (PF) theory. The simulated phase diagram composed of various coexistence regions involving single component mesophases (Cr1, Cr2, N2) and several coexistence phases (Cr1 + Cr2, Cr1 + N2, Cr1 + Cr2) accorded well with the experimental results. These predicted coexistence regions have been further confirmed by conducting several temperature quench experiments into these coexistence gaps by means of optical microscopy (OM). The development of phase morphology will be discussed in relation to the phase diagram.

1Supported by NSF-DMR 0514942 and REU DMR 0648318.

C1.00204 Multiscale Dynamics of Pre-Transitional Fluctuations in the Isotropic Phase of a Lyotropic Liquid Crystal1, MIKHAEL ANISIMOV, University of Maryland, College Park, CHRISTOPHER BERTRAND, The Petroleum Institute, Abu Dhabi, UAE, KIRT LINEGAR, University of Maryland, College Park, ANDREI KOSTKO, St. Petersburg State University of Refrigeration and Food Engineering, Russia — Using an improved static and dynamic light scattering technique, we have observed multiscale relaxation of the pre-transitional fluctuations in the isotropic phase of a cromolyn solution, a lyotropic liquid crystal where rods are formed by aggregates of disc-like molecules. We have detected the onset of cromolyn aggregation about 12 °C above the transition temperature. The onset is manifested by the emergence of strong scattering due to the fluctuations of local anisotropy and by the split of the diffusion dynamics into two modes, one associated with the diffusion of the cromolyn monomers and the other one with the diffusion of the cromolyn aggregates. A third observed dynamic mode is associated with the pretransitional slowing down of the fluctuations of local anisotropy. This mode behaves differently in polarized and depolarized light scattering, due to a coupling between the fluctuations of anisotropy and velocity fluctuations.

1The research is supported by Abu Dhabi National Oil and Gas Company, UAE.

C1.00205 Phase equilibria of a polymer discotic liquid crystal mixture.1, TSANG-MIN HUANG, THEIN KYU, University of Akron — Thermodynamic phase diagrams of a polymer dispersed liquid crystal (PDLC) containing a monomeric discotic liquid crystal (DLC) and a polymer have been established theoretically by combing Flory-Huggins theory for the free energy of mixing of isotropic phase and Chandrasekhar-Clark theory for the phase transition of hexagonal crystalline ordering of discotic liquid crystals. By varying interaction parameter of hexagonal columnar phase, columnar-isotropic and columnar-nematic-isotropic phase transitions can be predicted. The spinodal line of the columnar DLC/polymer will be calculated in conjunction with the conventional liquid-liquid spinodal. Effects of various molecular parameters on the columnar LC phase diagram will be discussed.

1Supported by NSF DMR 0514942.

C1.00206 Study of liquid crystal molecular dynamics algorithm1, JONES TSZ-KAI WAN, Department of Physics, The Chinese University of Hong Kong — Recent years have witnessed the growth in controlling liquid crystal (LC) alignment using patterned surfaces. Computer simulation of actual LC configurations that are due to different substrate surfaces is a useful tool to aid the design of practical LC cells. In liquid crystal simulations, one seeks for an optimal configuration of the LC director field n(r) that minimizes the total energy of the LC cell. For non-uniform substrate surfaces, the spatial variation of the LC is complicated and the minimization of the total energy is accomplished by advance numerical techniques like conjugate gradient (CG). In a recent work, we have proposed an efficient simulation scheme called liquid crystal molecular dynamics (LCMD), which is developed to determine liquid crystal configurations in complex physical environments. In this work, the author studies the limitation of such scheme and investigates how the simulation parameters can be tuned to achieve optimal performance.

1This work is supported by CUHK direct grant (project no. 2060307)

C1.00207 Atomistic DMD Simulations of Spontaneous Formation of Nematic and Smectic Phase in a Model Liquid Crystal.1, 2 APICHART LINHANANTA, Lakehead University, IAN MACKAY, University of Guelph — We present atomistic discontinuous molecular dynamics (DMD) simulations of the bulk liquid crystal phases of the molecular fluid 8CB. The model is based on previous DMD models of protein folding (A. Linhananta, J. Boer and Ian MacKay, J. Chem. Phys., 2005, 122, 114901) in which all atoms including polar hydrogen, but nonpolar hydrogen, are represented. Bonded pairs interact by infinite square well, while nonbonded atoms interact by hard-sphere square-well potentials. For the model 8CB, molecular parameters are scaled using AMBER and CHARMM force fields. The hard interaction potentials allow very rapid equilibration of ordered phases. Starting the DMD simulations from initial random states, without positional or orientation order, the 8CB systems spontaneously order nematic and smectic phases. The simulations were performed in a 40 A X 40 A X 40 A box with 100 to 500 8CB molecules. At fixed temperature, as the density increases, the phase change from disorder to nematic to smectic. Finally a density-strain phase diagram is presented.

C1.00208 An improved differential effective medium model for the viscosity of hard sphere suspensions at arbitrary volume fractions.1, 2 CARLOS MENDOZA, Materials Research Institute- UNAM, IVAN SANTAMARIA-HOLEK, Facultad de Ciencias-UNAM — We propose a simple and general model accounting for the dependence of the viscosity of a hard sphere suspension at arbitrary volume fractions. The model constitutes a continuum-medium description based on a recursive-differential method where correlations between the spheres are introduced through an effective volume fraction. In contrast to other differential methods, the introduction of the effective volume fraction as the integration variable implicitly considers interactions between the spheres of the same recursive stage. The final expression for the viscosity scales with this effective volume fraction which allows to construct a master curve that contains all the experimental situations considered. The agreement of our expression for the viscosity with experiments at low- and high-shear rates and in the high-frequency limit is remarkable for all volume fractions.

C1.00209 Adsorption energy of nanoparticles at liquid/liquid interfaces.1, KAN DU, E. GLOGOWSKI, T. EMRICK, T. RUSSELL, A. DINSMORE, Department of Physics, Department of Polymer Science and Engineering University of Massachusetts Amherst — We investigated the adsorption energy of nanoparticles at liquid/liquid interfaces by measuring the change of interfacial tension during the self-assembly of nanoparticles at interfaces. The sessile-droplet and pendent-droplet methods were used to measure the interfacial tension of liquid-gallium/water and oil/water interfaces. Interfacial tensions were measured under different conditions, including the concentrations and sizes of nanoparticles, ligand composition, solution pH, and ionic strength. The measurements showed that interfacial tension can change by an amount ranging from 0.5 to 150 mN/m. From the change in interfacial tension, we obtain the adsorption energy per nanoparticle, which ranges from less than 10 kBT to more than 1000 kBT. The results should contribute to the fabrication of membranes and other nano-composite materials by interfacial assembly.

1We acknowledge support from the NSF through NIRT CTS-0609107 and the Umass MRSEC on Polymers, and from the Center for UMass/Industry Research on Polymers.
C1.00210 Controlling Stability and Rheology of Organic Foams, JAMIE KROPIKA, MATTHEW CELINA, Sandia National Laboratories — It is often important to understand the stability and flow properties of polymeric foams in order to optimize industrial processing conditions or design new materials. The fact that foaming, polymerization and temperature rise are often coupled in these systems makes it difficult to even characterize existing materials, much less model behaviors to optimize formulations and processing conditions. To make progress in this area, we have developed model foaming systems that decouple these processes and allow us to characterize the physical properties of liquid foams. We are specifically interested in understanding the controlling factors of foam persistence, shear stability, and rheological behavior. We show both chemical (e.g., partial polymerization) and physical (e.g., particulate additives) means of tuning foam persistence as well as both small strain deformation flow and the less understood liquid-like flow at high applied stresses. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

C1.00211 Growth and self-assembly of water drops over evaporating polymer solutions, VIVEK SHARMA, Hatsopoulos Microfluids Laboratory (HML), Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge MA 02139., MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta GA 30332. — Water drops that nucleate and grow over evaporating polymer solutions exhibit non-coalescence and pack like hard spheres. In this study, we elucidate how the creation and evolution of a population of close packed drops occur in response to the heat and mass fluxes involved in water droplet condensation and solvent evaporation. We describe a rich array of experimental observations about water droplet growth, noncoalescence and assembly that have not been reported in the published literature so far. The pursuit of perfect packing in growing, assembling water drops is qualitatively similar to colloidal crystallization. We examine the role of solvent and polymer in controlling the kinetics of growth and assembly of droplets, which eventually evaporate away, producing a polymer film with ordered array of pores.

C1.00212 Molecular Dynamics of the Sedimentation of Polydisperse colloids, MANUEL VALERA, ATHULA HERAT, JOSEPH YARZEBINSKI, MARISA HICKS, Slippery Rock University — We have performed molecular dynamics simulation on colloidal systems composed of polydispersed hard spheres. The polydispersity in this systems had a Gaussian distribution with a range of up to 10%. We studied system where gravity plays a fundamental role. We show the sedimentation profiles and the effects on layering and crystallization for different values of the gravitational length, polydispersivity and area density of the system.

C1.00213 Gradient Sensing in Reactive, Ternary Membranes, OLGA KUKSENOK, ANNA C. BALAZS, University of Pittsburgh — Using computer simulations, we investigate the behavior of reactive ternary ABC membranes that are subjected to an external, spatially nonuniform stimulus, which controls the rate of interconversion between the A and B components. We assume that A and B have different spontaneous curvatures. Furthermore, the C component is taken to be nonreactive and incompatible with both A and B. We find that a gradient in the applied stimulus causes the dynamic reconstruction of the membrane, with a preferential reorientation of the reactive AB domains along the gradient. In addition, the external gradient effectively controls the transport of the nonreactive C component within the membrane. The latter effect could potentially be exploited for cleaning the membrane of the nonreactive C impurities or for the targeted delivery of the C component to specific locations.

C1.00214 Line Tension and the Nature of the Boundary in a Pure Model System, RICHELLE TEELING, PRITAM MANDAL, LU ZOU, Kent State University, ANDREW BERNOFF, Harvey Mudd College, JAMES ALEXANDER, J. ADIN MANN, Case Western Reserve University, ELIZABETH MANN, Kent State University — Insoluble 8CB (4-n-octyl-4-cyanobiphenyl) layers at the air/water interface provide a well-controlled system on which to analyze the line tension and the nature of the boundary between quasi-two dimensional domains. The average molecular area was adjusted to monolayer liquid/gas or to monolayer/trilayer coexistence. In the first case, difference in dipole moment density leads to long-range repulsive forces which affect line tension and domain configuration. The symmetry of additional bilayers in the second system minimizes such effects, allowing a direct test of the effect of repulsive forces. The line tension of both systems was determined from the hydrodynamic relaxation of stretched domains, through quantitative comparisons with a numerically tractable hydrodynamic model for the relaxation. This research will give insight into similar system of lipids and proteins in biological membranes.

C1.00215 Mesoscopic Simulations of Microfluidic Flow in Irregular Geometries, TYLER N. SHENDRUK, GARY W. SLATER, University of Ottawa — Stochastic Rotation Dynamics, a particle-based model for mesoscopic fluid dynamics, is used to study two and three-dimensional flow in a variety of complex boundaries and for a range of low Reynolds numbers (between 10 and 200). The systems considered are of two types: they consist of either irregular geometries such as dimpled pipes or require adaptive boundary conditions such as particle impact on a solid boundary. We apply out techniques to microfluidic devices with complex channel walls such as those used for slalom chromatography and sinusoidal undulation surface patterning chromatography. Numerical results showing good agreement with experimental data and previous computational simulations are presented.

C1.00216 Polymer Brushes Driven by Electro-Osmotic Flow in Nanoscale Channels, IBRAHIM SOUKI, MOHAMED LARADJI, University of Memphis, P.B. SUNIL KUMAR, IIT-Madras — Using systematic dissipative particle dynamics simulations, we investigated the flow of solvents in nanoscale channels, driven by wall grafted polyelectrolytes, under the influence of an oscillating external electric field. Net flow of the fluid is observed when the external field is temporally asymmetric. We found that the flow rate is strongly affected by grafting density, chain length, field amplitude and period. In particular we can achieve an optimum flow rate for specific values of the parameters listed above. The details of polymer kinetics involved and their effect on net fluid flow will be presented.

C1.00217 Guiding E.coli to nanosensors, DONG-WON PARK, HYE-MI SO, KRICT, BEOM SOO KIM, Chungbuk National University, KI-JEONG KONG, HYUNJU CHANG, JEONG-O LEE, KRICT — Electronic nanosensors based on nanomaterials such as carbon nanotubes and nanowires are expected to have ultimate sensitivity. However, as an inherent problem of nanosensors, they have extremely small sensor surface for reaction. Therefore, simple diffusion of target biomolecules is not enough for such nanosensors, and the problem is even more serious in the case of motile bacteria. Previously, we have shown that we could estimate the titer of E.coli with arrays of single-walled carbon nanotube field effect transistors (SWNT-FET) combined with statistical method. Still, sensitivity of our method is inferior compared with incubation method, due to the limited sensor surface area. In this work, we actively guide E.coli to the sensor surface using micro-fabricated channels. Arrow-shaped and funnel shaped microstructures were fabricated in the channel to guide E. coli to the sensor surface, and we used green fluorescent protein expressed E.coli to monitor the guiding of E.coli.
C1.00218 Hydrodynamic flow in a microchannel due to nanocapillary membrane electro-osmotic flow. JARROD SCHIFFBAUER, Physics Dept., West Virginia University, WILL BOOTH, Physics Dept., West Virginia University, KATHLEEN KELLY, Chemistry Dept., West Virginia University, BOYD EDWARDS, Physics Dept., West Virginia University, AARON TIMPERMAN, Chemistry Dept., West Virginia University — A model for hydrodynamic flow in a microchannel terminated by a nanocapillary membrane (NCM) is proposed in which the microchannel electric-double layer (EDL) is treated as a boundary-layer, providing a hydrodynamic slip-velocity at the channel wall, and the NCM electro-osmotic flow (EOF) is treated as fully-developed. Applied pressure gradients and the contribution of the microchannel EDL to both the net charge transport and the back-pressure on the NCM are neglected. The proposed coupling between the NCM EOF and microchannel hydrodynamic response is obtained by arguing that the steady-state Onsager symmetry between linear-response coefficients may be applied to the transient response of the microchannel. The resulting form of the Navier-Stokes equation in the microchannel possesses steady-state solutions that are compatible with parabolic and inverted-parabolic profiles observed in NCM sample concentration experiments.

C1.00219 Measurements of Stopping Force on Ball on Impact with Granular Medium. JOSEPH AMATO, LAURA COYLE1, MICHAEL NITZBERG2, Colgate University — We present direct measurements of the deceleration vs. time of a 3.8 cm diameter brass ball plunging into a loose granular bed of 400 - 600 μm glass beads. Data were obtained using an accelerometer chip housed within the ball. As suggested by Durian and co-workers, the measured force on the ball is well described by a velocity dependent force \( c_1 \nu^3 \) plus a separate depth dependent force \( c_2 (z + z_0) \). For impact velocities in the range 1.3 – 5.1 m/s, a single set of parameters \((c_1, c_2, z_0)\) fits all the data well, with the exception of the first few ms after impact, when the ball is only partially submerged in the granular matter.

1 undergraduate
2 undergraduate

C1.00220 Fluidization of granular media wetted by liquid \( ^4 \text{He} \). KAI HUANG, MASoud SOHAILI, MATTHIAS SCHROETER, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-organization — We explore experimentally the fluidization of vertically agitated PMMA spheres wetted by liquid \( ^4 \text{He} \) at temperatures around the \( \lambda \) point. For wetting by normal fluid helium \((T > T_\lambda)\), the critical acceleration for fluidization \((\Gamma_c)\) shows a steep increase close to the saturation of the vapor pressure in the sample cell. For superfluid helium \((T < T_\lambda)\) wetting, \( \Gamma_c \) starts to increase already at about 75% saturation, indicating that capillary bridges are enhanced by the superflow of unsaturated helium film driven by “fountain effect”. Above saturation, \( \Gamma_c \) enters a plateau regime where the capillary force between particles is independent of the bridge volume. The plateau value is found to vary with temperature and shows a peak at 2.1 K, which we attribute to the influence of the specific heat of liquid helium on capillary bridge formation and rupture.

C1.00221 Melting in a finite, two-dimensional Yukawa system. T.E. SHERIDAN, Ohio Northern University — A complex (dusty) plasma disk is a two-dimensional system of monodisperse microspheres confined by a parabolic well and interacting through a Yukawa potential. (Complex plasma is an open, dissipative system.) Consequently, a complex plasma disk is a physical realization of a finite, two-dimensional Yukawa system. Recent experiments on a complex plasma disk with \( n \approx 3900 \) dust particles [T. E. Sheridan, Phys. Plasmas 15, 103702 (2008)] indicate that the system melts via two second-order topological phase transitions. In the present work, we will model these experimental results using the Metropolis algorithm to generate ensembles of configurations consistent with a given thermodynamic temperature. Model results will be compared with experiment. In particular, we wish to determine the exponential characterizing the power law decay of the bond-orientational correlation function in the hexatic phase, which the experimental results indicate may be greater than that predicted by KTHNY theory.

C1.00222 Percolation in Granular Material. MARK ZIMMERMAN, D.T. JACOBS, Department of Physics, The College of Wooster, Wooster OH 44691 — Percolation was studied by measuring the resistance to the flow of electricity through a system of conducting and insulating spheres. The percolation threshold was measured on three different size systems by varying the number fraction of conducting spheres in the mixture of 3 mm diameter steel shot and glass spheres as well as 1 mm silver coated glass spheres and uncoated spheres. A dynamic pressure effect was observed in the random-packed system when using the less conducting steel shot but not with the silver coated spheres. Results have qualitative and quantitative similarities to published experimental and simulation work on comparable systems going from 2D to 3D. The percolation threshold observed will be discussed and compared to other experiments as well as simulations. We acknowledge support from NSF DMR-0649112.

C1.00223 Self-Organized Criticality in a Bead Pile. MIKE WINTERS, D.T. JACOBS, Department of Physics, The College of Wooster, Wooster OH 44691 — This experiment examined a conical bead pile and the distribution of avalanche sizes when using uniform 3mm zirconium spheres ("beads"). A bead pile is built by pouring beads onto a circular base where the bottom layer of beads had been glued randomly. Beads are then individually dropped from a fixed height after which the pile is massed. This process is repeated for thousands of bead drops. By measuring the number of avalanches of a given size that occurred during the experiment, the resulting distribution could be compared to a power law description as predicted by self-organized criticality. We had found in an earlier experiment that glass beads dropped from a small height were consistent with a simple power-law, but if dropped from larger heights then a power-law times an exponential was needed. The zirconium beads sometimes had a distribution that deviated from a power-law times an exponential when the beads were dropped from larger heights, and occasionally the distribution showed a distinct enhancement of the probability for large avalanches when beads were dropped from smaller heights. Using data collected over many years, it was found that the density and type of bead did not appear to affect the avalanche distribution. We compare our experimental results to a numerical simulation. We acknowledge support from NSF DMR-0649112.

C1.00224 The mussel thread cuticle, a biological granular composite coating. NIELS HOLTER-ANDERSEN, University of Chicago, Department of Chemistry, Chicago, IL 60637, USA, HEÑRIK BIRKEDAL, University of Aarhus, Department of Chemistry & iNano, 8000 Aarhus C, Denmark, KAA YEE C. LEE, University of Chicago, James Franck Institute, Chicago, IL 60637, USA. J. HERBERT WAITE, University of California, Santa Barbara, Biomolecular Science & Engineering Program, Santa Barbara, CA 93106, USA — The cuticle of mussel byssal threads is a peculiar natural granular composite coating that combines high extensibility with high stiffness and hardness. In this study fluorescence microscopy and elemental analysis were exploited to show that the 3, 4-dihydroxyphenyl-L-alanine (dopa) residues of mussel foot protein-1 co-localize with Fe and Ca distributions in the cuticle of Mytilus galloprovincialis mussel byssal threads. Removal of Fe and Ca from the cuticle by chelation results in a 50% reduction in hardness. Dopa-metal complexes may be a significant source of stability as cross-links in the composite cuticles.
C1.00225 Electron Shock Waves Propagating into a Pre-ionized Medium , M. HEMMATI, N. RASUL, R. PEDEN, Arkansas Tech University — We employ a one dimensional, constant velocity, steady-state, three component fluid model to investigate breakdown waves propagating into an ionized medium. Assuming that electron gas partial pressure is much greater than that of the other species, we have been able to write down equations of conservation of the flux of mass, momentum and energy, plus the Poisson’s equation. The charge concentration ahead of the wave alters the set of fluid equations and also the boundary conditions at the shock front. The ionization rate is calculated by considering ionization from both random and directed electron motions. Integration of the set of electron-fluid dynamical equations for antiforce waves propagating into a pre-ionized medium through the dynamical transition region of the wave for two wave speeds and several current values ahead of the wave was successful. The results for both wave speed values and all current values ahead of the wave meet the expected physical conditions at the end of the sheath region. Calculation of the ionization rate through the sheath region shows that for high wave speeds and for all current values ahead of the shock front, as one approaches the trailing edge of the sheath, the ionization rate increases slightly. However, as the wave speed decreases, for all current values ahead of the shock front, the ionization rate essentially remains constant throughout the sheath region.

C1.00226 Bubble Chains in Magnetic Fluids (Ferrofluids). JONG(JAMES) YOO1, PHILIP YECKO, Montclair State University, WAH-KEAT LEE. Advanced Photon Source – Argonne National Laboratory — Direct numerical simulations are applied to the problem of dynamics of chain formation among small bubbles in a magnetic liquid (ferrofluid), coalescing at low Reynolds number due to magnetophoresis. Complementary experiments performed using high-intensity high-resolution X-ray images of air bubbles in ferrofluid have revealed that linear chains of several small bubbles are extremely common. In numerous applications of ferrofluids, the wanted or unwanted presence of bubbles and bubble chains in particular, is crucial to describing and predicting critical flow properties. In this study we examine the chain formation process between two and three identical bubbles, finding regimes of conditions within which chain formation is expected under a uniform applied magnetic field. We conjecture how these results can be extended to larger numbers of bubbles forming longer chains. Added mass plays a significant role in the magnetophoresis-driven dynamics. We therefore examine the role of the density ratio in the coalescence process among bubbles within the limits imposed by the volume of fluid (VOF) method that we use.

1Undergraduate student

C1.00227 Charge transport mechanism of ionic liquids at metallic interfaces , ANATOLI SERGHEI, University of Massachusetts Amherst, MARTIN TRESS, JOSHUA RUME, FRIEDRICHER KREMER, University of Leipzig, Germany — A quantitative description is suggested for electrode polarization, an ubiquitous phenomenon which takes place at the interface between a metallic and an ionic conductor. Based on the fact that, due to Coulombic interactions, the ion mobility is drastically slowed down at the interfaces, this approach quantitatively describes the experimentally observed scaling laws and enables one to deduce – by use of a novel formula – the bulk conductivity of the ionic charge carriers under study. It allows furthermore a quantitative determination of the conductivity function of the ionic liquids in the interfacial regions and opens, by that, multiple perspectives in understanding the mechanisms of charge transport at interfaces.

C1.00228 Exact thermodynamic calculation of a monatomic system and its ideal glass transition on a new recursive lattice formed by cubic units , RAN HUANG, PURU GUJARI, The University of Akron — A many-body Ising lattice model is used to represent monatomic systems and is solved exactly on a new recursive lattice with the aim to study the metastability in supercooled liquids and the ideal glass transition. Interactions between particles farther away than the nearest neighbor distance are taken into consideration. The Ising model is antiferromagnetic in nature so that its ordered phase represents an alloy-type crystal of alternating species (A-B or particle-void). The new recursive lattice appears quite reliable to represent a cubic lattice. Thermal properties including free energy, energy and entropy of the ideal crystal and supercooled liquid state of the model are calculated. The computation results show a first order melting and second order ideal glass transition (entropy crisis) in the supercooled liquid phase. The effects of different energy terms on the two transitions are studied. We also study the defects in the ideal glass, supercooled liquid and the crystal to support the theory that a glass can be treated as a highly defective crystal.

C1.00229 Pattern formation in two-dimensional binary mixtures of colloids interacting via short-ranged interactions , CARLOS MENDOZA, ERASMO BATTA, Materials Research Institute-UNAM — We report Monte Carlo simulations on the pattern formation in a binary mixture of colloidal particles interacting via short ranged potentials. Such potentials consist of a hard-core square-shoulder interaction if the particles are of the same type and of a hard-core square-well if they are of different type. For 50/50 mixtures, we find a rich variety of patterns that can be grouped mainly in alternate strips each one consisting of particles of the same type or aggregates that self-assemble in a regular square lattice. For mixtures in which the are more particles of one of the species then a phase separation is observed; one of the separated phases consists only of particles of the dominant type while the other is a mixture of both types of particles.

C1.00230 ABSTRACT WITHDRAWN –

C1.00231 Phase Separation in the Advective Cahn-Hilliard Equation with a Chaotic Flow , SOHEI YASUDA, BENJAMIN VOLLMAYR-LEE. Bucknell University — The phase separation between two immiscible liquids advected by a chaotic flow is studied by numerical simulations of the advective Cahn-Hilliard Equation. It has been shown that the competition between phase separation dynamics, which tends to grow domains, and chaotic flow, which tends to break up the domains, determines the length scale characterizing the domains in the steady state. We extend this analysis to investigate the correlation between the local finite-time Lyapunov exponent field and the domain structure. In particular, we consider alternating sine flows and an alternating periodic vortex flow. We also investigate whether the steady state domain structure demonstrates any history dependence by studying both a initially mixed state and an initially phase separated state. A summary of our results is presented.


C1.00232 Controlling Pattern Formation in Polymer and Nanoparticle Assemblies via Programmed Flow-coating , HYUN SUK KIM, MARK MCDONOUGH, SAM PENDERGRAPH, ALFRED CROSBY, Polymer Science and Engineering Department, University of Massachusetts — We have developed a novel flow-coating method for assembling periodic polymer and nanoparticle line patterns with controlled spacing and width of lines. In flow-coating, a dilute polymer and/or nanoparticle solution is held by capillary forces under a stationary knife blade fixed at gap height above a substrate fixed to a translating stage. Upon translating the substrate, spontaneous formation of convective polymer and nanoparticle assemblies occurs at the three-phase contact line of the meniscus. We demonstrate that the width and spacing of deposited lines can be controlled over a wide range by using programmed velocity profiles for the translating stage. Deposition of solutes is induced when contact lines are “stick” at slow or zero velocity, while limited deposition occurs during “slip” at high velocity. We investigate the effect of gap height, concentration, and velocity on the pattern formation. This new method provides an easy, robust, and lithography-free method to control the deposition of line pattern of polymers and nanoparticles for various applications.
C1.00223 Nonlinear I-V Characteristics of Nano-Pores: Depletion Layer Pattern Formation and Vortex Instability . GILAD YOSSIFON, HSUEH-CHIA CHANG, University of Notre Dame — We report the first direct experimental proof for Rubinstein’s instability [1] by using an applied AC electric field across a straight nano-pore, whose transverse dimension is at least 10 times larger than the depletion layer, EO convective flow is completely arrested and ion transport is dominated by diffusion and electro-migration. The ion flux dynamics is imaged using fluorescent dye molecules in combination with confocal microscopy, to understand the non-equilibrium phenomenon of over-limiting current density across a nanoporous membrane. With a slow AC field, an ion depletion front is generated intermittently from one end of the nano-slot and a vortex instability is found to arrest the self-similar diffusive front growth. This electrokinetic instability evolves into a stationary interfacial vortex array that specifies the over-limiting current, independent of external stirring or convective flow. [1] I. Rubinstein, E. Staude and O. Kedem, Desalination 69, 101 (1988).

C1.00224 Transfer of colloidal particles using the reversible buckling patterns . DONG CHOON HYUN, UNYONG JEONG, Department of Material Science and Engineering, Yonsei University, Seoul, Korea — Buckling or wrinkling is a well-known phenomenon. It is realized by releasing strain applied to a hard film on an elastomer substrate. Strain engineering allows the buckling to have the highly ordered and regular wavy surfaces. The amplitude of the buckling can be reversibly tuned by a cycle of applying and releasing strain. This reversible nature of buckling was used to deposit the spherical colloids in the trenches of the wavy patterns and transfer the colloids to flat surfaces. The colloidal deposition and transfer was repeatedly carried out to fabricate identical patterns of colloidal assembly. In this presentation, we will demonstrate complex colloidal patterns (hydrogels colloids, silica, Au nanoparticles, magnetic nanoparticles) transferred from the buckled surfaces.

C1.00225 DNA Linker Mediated Assembly of Colloidal Nanoparticles1 . HUIMING XIONG, DANIEL VAN DER LEIE, OLEG GANG, Brookhaven National Laboratory — When flexible ssDNA linkers are added to the mixture of two types of dispersed, ssDNAs capped gold nanocolloids which are mutually non-complementary but complementary to the respective ends of the linker DNA, a crystalline phase of body-centered-cubic unit cell forms. The phase diagram of DNA linker mediated nanoparticle assemblies has been experimentally investigated and constructed by using in-situ small angle x-ray scattering. The influence of linkage defects on crystalline structure was also examined.

1Research was supported by the U. S. DOE Office of Science and Office of Basic Energy Sciences under contract No. DE-AC-02-98CH10886.

C1.00226 Birefringence Measurements of Spherulites formed in β-Lactoglobulin . ERIC HARDIN, BRAD KIRKWOOD, JAZMINE LOMAN, ATHULA HERAT, Slippery Rock University, RIZWAN MAHMOOD, Slippery Rock University, KRISTIN DOMIKE, Wooster College — Many proteins have a propensity to aggregate into amylloid fibril containing spherulite-like structures. In some instances these spherulitic protein aggregates have been observed in people suffering from a number of neurodegenerative diseases, including Alzheimer’s, Parkinson’s, and Creutzfeldt-Jakob’s. However, the exact role these aggregates play in the body, their internal structure, and the aggregation mechanism still remains a mystery. The model protein used in our study, β-lactoglobulin (BLG), produce spherulites under low pH and high temperature conditions. We report birefringence measurement on BLG using phase retardation method as a function of temperature. Birefringence (−0.0022 ± 0.0002) data suggest very weak ordering within the spherulites. These spherulites seem to disappear when we added an extensively studied thermotropic liquid crystal [4’-pentyl-4-cyanobiphenyl (SCB)] in β-Lactoglobulin + water + hydrochloric acid. Our preliminary data suggests that the strong interaction energy between the two systems may lead to the destruction of spherulites.

C1.00227 Solvation structure of ice-binding antifreeze proteins . HENDRIK HANSEN-GOOS, JOHN WETT-LAUFER, Department of Geology and Geophysics, Yale University — Antifreeze proteins (AFPs) can be found in organisms which survive at subzero temperatures. They were first discovered in polar fishes since the 1950’s [1] and have been isolated meanwhile also from insects, plants, and bacteria. While AFPs shift the freezing point of water below the bulk melting point and hence can prevent recrystallization, the effect is non-colligative and there is a pronounced hysteresis between freezing and melting. For many AFPs it is generally accepted that they function through an irreversible binding to the ice-water interface which leads to a piecewise convex growth front with a lower nonequilibrium freezing point due to the Kelvin effect. Recent molecular dynamics simulations of the AFP from Choristoneura fumiferana reveal that the solvation structures of water at ice-binding and non-ice-binding faces of the protein are crucial for understanding how the AFP binds to the ice surface and how it is protected from being overgrown [2]. We use density functional theory of classical fluids in order to assess the microscopic solvent structure in the vicinity of protein faces with different surface properties. With our method, binding energies of different protein faces to the water-ice interface can be computed efficiently in a simplified model. [1] Y. Yeh and R.E. Feeney, Chem. Rev. 96, 601 (1996). [2] D.R. Nutt and J.C. Smith, J. Am. Chem. Soc. 130, 13066 (2008).

C1.00228 Hovering of a free rigid pyramid in an oscillatory air flow . BIN LIU, NYU, BRENDAN FOLIE, HMC, ANNIE WEATHERS, JUN ZHANG, STEPHEN CHILDRESS, NYU — We investigate the dynamics of free rigid bodies when moving in an oscillating background flow. Given a pyramid-shaped object, the fluid drag due to a downward flow and an upward flow around the body differ when the inertia of the air flow is relevant. We find that when the amplitude of the air flow is above a threshold, the net lift on the pyramid overcomes its weight. The body then starts to hover, despite the fact that the air flow has no upward or downward preference. The threshold amplitude of the oscillating air depends on the weight of the rigid object and its geometric anisotropy. We show that at a given frequency there is an optimal shape of the pyramid, such that hovering occurs at minimal amplitude of the flow.

C1.00229 ABSTRACT WITHDRAWN —

C1.00240 GENERAL PHYSICS —

C1.00241 Mass, Energy, Space And Time System Theory—MEST A way to help our earth . DAYONG CAO, Beijing Natural Providence Science & Technology Development Co., LTD — There are two danger to our earth. The first, the sun will expand to devour our earth, for example, the ozonosphere of our earth is be broken; The second, the asteroid will impact near our earth. According to MEST, there is a interaction between Black hole (and Dark matter-energy) and Solar system. The orbit of Jupiter is a boundary of the interaction between Black hole (and Dark matter-energy) and Solar system. Because there are four terrestrial planets which is mass-energy center as solar system, and there are four or five Jovian planets which is gas (space-time) center as black hole system. According to MEST, dark matter-energy take the velocity of Jupiter gose up. So there are a lot of asteroids and dark matter-energy near the orbit of Jupiter-the boundary. Dark matter-energy can change the orbit of asteroid, and take it impacted near our earth. Because the Dark matter-energy will press the Solar system. It is a inverse process with sun’s expandedness. So the “two danger” is from a new process of the balance system between Black hole (and Dark matter-energy) and Solar system. According to MEST, We need to find the right point for our earth in the “new process of the balance system.”
C1.00244 Green Energy - Fiction and Reality, LAWRENCE CRANBERG, Texas Fireframe Co. — The term “Green Energy” has been popularized to refer to energy sources that do not depend on fossil fuels. The oldest truly “green” energy source is wood fuel derived by photosynthesis for thermal comfort in the cold season. Thermal energy from the combustion of wood for personal heating in our 41 million fireplaces has greatly declined, due to an “Anti-fireplace Hoax” (1) that fireplaces are “energy counterproductive.” Physicists have a special obligation to address the problem that our major true source of “Green Energy” is widely misrepresented and neglected. 1. L. Cranberg, The Physics Teacher, Letter, January,1989

C1.00245 Biothermophotonics evaluation of multilayered tissue structures, ANNA MATVIENKO, ANDREAS MANDELSI, University of Toronto, Canada, STEPHEN ABRAMS, Quantum Dental Technologies Inc, Toronto, Canada — Biothermophotonics is a novel non-invasive method for safe in vivo evaluation of thermal and optical properties of tissues. The method involves analysis of photothermal field induced in a sample by frequency-modulated laser excitation and following optical-to-thermal energy conversion. The theoretical model for fitting the properties of the sample features coupled diffuse-photon-density-wave and thermal-wave mathematical description. The sample is considered to be a multilayered one-dimensional structure. The best fits to the model are obtained with Simplex Downhill algorithm for multi-parameter minimization. The results demonstrated robustness of the algorithm and the capabilities of the method to simultaneously evaluate optical and thermal properties of multilayered tissue structures in vivo.

C1.00246 STATISTICAL AND NONLINEAR PHYSICS –

C1.00247 Excursion time distributions of heartbeat time series, ISRAEL REYES-RAMIREZ, LEV GUZMAN-VARGAS, Instituto Politecnico Nacional - UPITTA, Mexico — We present a study of heart interbeat time series based on excursion time distributions from healthy subjects and patients with heart failure. We describe some differences between these groups by means of the calculation of the characteristic time scale of the exponential distributions for stationary segments. We also compare day-night periods for both groups. In particular, we find that the characteristic time scale associated to the healthy group is slightly smaller than the heart failure group, indicating that large excursions are more probable under pathologic conditions. When day-night period are compared, we observe that night records lead to a smaller time constant than day records. Moreover, we simulate correlated noises with power spectrum of the form $S(f) \sim f^{-\beta}$ with $0 < \beta < 1$, to detect changes in the excursion time distributions with the presence of long-range correlations. Finally, we discuss our results in the context of heartbeat dynamics.

C1.00248 Mittag-Leffler Correlated Noise and Anomalous Diffusion within a Single Protein Molecule, KE-GANG WANG, Department of Physics and Space Sciences, Florida Institute of Technology, Melbourne, FL 32901, DANIEL VIÑALES, JOSÉ HOYOS, Duke University — The effects of quenched disorder on nonequilibrium phase transitions in the directed percolation universality class are revisited. Using a strong-disorder energy-space renormalization group, it is shown that for any amount of disorder the critical behavior is controlled by an infinite-randomness fixed point in the universality class of the random transverse-field Ising models. The experimental relevance of our results are discussed.

Financial support: NSF

C1.00249 Contact process with sublattice symmetry breaking, RONALD DICKMAN, UFMG, MARCELO MARTINS DE OLIVEIRA, Universidade Federal de Vícosa — We study the phase diagram and scaling properties of a contact process with creation at first- and second-neighbor sites and inhibition at first-neighbors. Inhibition takes the form of an increased annihilation rate, proportional to the number of occupied neighbors of a given site. The pair approximation predicts the existence of three phases, inactive (absorbing), active symmetric, and active asymmetric, the latter exhibiting distinct sublattice densities on a bipartite lattice. These phases are separated by continuous transitions in the space of control parameters; the pair approximation is reentrant. Monte Carlo simulations in two dimensions verify the existence of a phase with broken sublattice symmetry. The symmetric-asymmetric transition appears to belong to the Ising universality class, as expected from symmetry considerations.

1DMR-0804107

C1.00243 PAW dataset library for the Quantum-Espresso package, RASHID HAMDAN, CHAO CAO, University of Florida — The frozen-core approximation is widely employed in plane-wave density functional theory calculations, because it can greatly reduce the required cut-off energy to achieve convergence. The commonly used ultra-soft pseudopotential method is one flavor of this approximation. Despite its advantages, the ultra-soft pseudopotentials are difficult to generate, and it is difficult to control the quality. It is also impossible to reconstruct the complete wave functions from the pseudopotential method calculations. The PAW method was developed to conquer these difficulties. We have constructed a set of soft, reliable PAW dataset library for the Quantum-Espresso package. The datasets were thoroughly tested, and the results were compared with VASP calculations. As a demonstration, we present the comparison with VASP calculations for Bromine doped graphite system and a comparison between the ultra-soft pseudopotential and PAW calculations of the recently discovered iron-based superconductor LaFeAsO compound. The PAW calculations yielded magnetic moment that is much closer to experimental value than the ultra-soft pseudopotential calculations.

C1.00242 On the Earthly Origin of the Penzias-Wilson Microwave Background, DMITRI RABOUNSKI, LARISSA BORISSOVA — According to the experimental analysis conducted by P.-M. Robitaille, the 2.7K microwave background, first detected by Penzias and Wilson, is not of cosmic origin, but of the Earth, and is generated by oceanic water. With these we have two entire fields to consider (Robitaille, Progr. Phys., 2007, v. 4, 74): (1) the Earth Microwave Background, the EMB, present with the 2.7K monopole and 3.5mK dipole components; (2) the weak (micro Kelvins) Intergalactic Microwave Background, the IMB, which is connected to the entire Metagalaxy. This conclusion meets our theory. First, the field density of the EMB, being inversely proportional to the field volume, should decrease with the cube of the distance from the Earth’s surface, while its dipole anisotropy, which is due to the motion of the entire field in common with the Earth, is independent from altitude. Therefore the EMB monopole shouldn’t be found at the 2nd Lagrange point (far distant from the Earth), while the dipole anisotropy remained the same that near he Earth. Second, Einstein’s equations for commonly the EMB and the IMB are valid only if the Metagalaxy’s entire space rotates, that permits some cosmological conclusions.
C1.00251 Absorbing-state transitions on percolating lattices, MAN YOUNG LEE, THOMAS VOJTA, Missouri University of Science and Technology — We study the nonequilibrium phase transitions of reaction-diffusion systems into absorbing states. In the presence of quenched disorder, i.e., spatial impurities or defects, the interplay between geometric and dynamical fluctuations leads to exotic behavior and ultraslow dynamics. Specifically, we investigate the contact process on a randomly diluted lattice. We find that the nonequilibrium phase transition across the percolation threshold of the lattice is characterized by unconventional activated (exponential) dynamical scaling and strong Griffiths effects. We calculate the critical behavior in two and three space dimensions, and we relate our results to the infinite-randomness fixed point in the disordered one-dimensional contact process. To confirm the universality of this exotic scaling scenario we also study generalizations of the contact process involving several absorbing states, and we support our calculations by Monte-Carlo simulations.

C1.00252 Infinite-randomness critical point in the two-dimensional disordered contact process, ADAM FARQUHAR, JASON MAST, THOMAS VOJTA, Missouri University of Science and Technology — We study the nonequilibrium phase transition in the two-dimensional contact process on a randomly diluted lattice by means of large-scale Monte-Carlo simulations for times up to $10^{10}$ and system sizes up to $8000 \times 8000$ sites. Our data provide strong evidence for the transition being controlled by an exotic infinite-randomness critical point with activated (exponential) dynamical scaling. We calculate the critical exponents of the transition and find them to be universal, i.e., independent of disorder strength. The Griffiths region between the clean and the dirty critical points exhibits power-law dynamical scaling with continuously varying exponents. We discuss the generality of our findings and relate them to a broader theory of rare region effects at phase transitions with quenched disorder. Our results are of importance beyond absorbing state transitions because according to a strong-disorder renormalization group analysis, our transition belongs to the universality class of the two-dimensional random transverse-field Ising model.

C1.00253 Efficiency, coherent transport and entropy fluctuations in a Brownian motor driven by time-dependent temperature, RONALD BENJAMIN, University of Alabama at Birmingham — We investigate the transport and energetics of a Brownian motor driven by position dependent temperature. We found that coupling enhances the current as well as the efficiency. Novel features such as current reversal with respect to the coupling strength and inertia of the Brownian particle is also observed. We also find that the total entropy production satisfies the fluctuation theorem in the steady state.

1 I thank the University of Alabama, Birmingham Graduate school for GAFP Fellowship

C1.00254 Unified approach to the derivation of work theorems for equilibrium and steady-state, classical and quantum Hamiltonian systems, DANIEL KOSOV, University of Maryland, MAXIM GELIN, TU Munich — The fluctuation theorems rigorously relate equilibrium ensemble properties of a dynamical system with its evolution under nonequilibrium conditions, beyond the domain of validity of the linear response theory. We present a unified and simple method for deriving work theorems for classical and quantum Hamiltonian systems, both under equilibrium conditions and in a steady state. We adopt the partitioning of the total Hamiltonian into the system part, the bath part, and their coupling. We derive many equalities which are available in the literature and obtain a number of new equalities for nonequilibrium classical and quantum systems. Our results can be useful for determining partition functions and generalized free energies through simulations or measurements performed on nonequilibrium systems. We derive a semiclassical version of the work theorem and discuss the definition of semiclassical work operator. Phys.Rev. E 78, 011116 (2008)

C1.00255 On the quantum master equations for BCS-type quasiparticles, C.F. HUANG, CMS/ITRI, K.-N. HUANG, Institute of Atomic and Molecular Sciences, Academia Sinica — The quantum master equations are introduced for the density matrices of BCS-type quasiparticles, which may include both the particle-particle and particle-hole couplings. The constraints to relate the loss and gain factors are important to preserve the forms of the density matrices under such equations. These two factors describe not only the scattering where the number of quasiparticles are conserved, but also the creation and destruction of quasiparticles. The introduced equations can be reduced to the semiclassical master equations in the homogeneous limit.

C1.00256 Obtaining the fractal dimensions and length distributions for the external hulls of Q-state Potts model clusters, DAVID ADAMS, LEONARD SANDER, ROBERT ZIFF, University of Michigan — We obtain the fractal dimensions of the complete and external hulls of Q-state Potts model clusters. We grow percolation clusters (Q=1) using the Leath method. For Q>1 up to the upper critical dimension (Q=4), we grow Fortuin-Kasteleyn (FK) clusters using the Swendsen-Wang method. Our results for fractal dimension for the complete and external hulls agree with the predictions of Duplantier. We also obtain the distribution of complete and external hull lengths and cluster height. For a given Q, the distributions for different size systems can be collapsed using scaling. The distributions of heights display simple exponential tails, which can be understood in terms of hull walks and the geometry of the system.


C1.00258 The Role of Walls’ Stochastic Forces in Statistical Mechanics – Irreversibility and Transition from One Microstate to Large Number of Microstates, MADHAV GAUTAM, PURU GUJRATI, The University of Akron — A statistical system, by definition, experiences uncontrollable stochastic interactions with the surrounding and allow for irreversibility. A purely deterministic system will not show any irreversibility. One can model the walls of the container containing a system to be the source of these stochastic impulses. We present the results of such stochastic walls’ impulses on a single particle in a one-dimensional box of a fixed length. At each collision with the walls, the velocity changes due to stochastic impulses so that the velocity becomes unpredictable. After a long period of time, a single initial velocity results in a distribution of velocities. If the strength of the impulse is not too strong, the average kinetic energy reaches a finite limit, so that it can be used to define the temperature.


C1.00259 Lack of Molecular Chaos and the Role of Stochasticity in Kac’s Ring Model, PRADEEP FERNANDO, PURU GUJRATI, The University of Akron — The dynamics of a system can either be deterministic or stochastic. In deterministic dynamics, there is unique one-to-one relationship between the initial state of the process and its evolution at a later time, while in stochastic process, there are several possible outcomes or evolved sates in future. Since the outcome is not certain, we use one-many relationships between the current states and its evolution in future. We use simple Kac ring model to demonstrate the properties of deterministic and stochastic dynamics. The results lead us to understand the following: 1) In deterministic dynamics, a system always has a unique equilibrium state with zero fluctuation. Instead, the initial state recurs eventually following Poincare Recurrence. In particular, molecular chaos assumption of Boltzmann cannot be justified. 2) In stochastic dynamics the system reaches equilibrium irrespective of the initial state. References: [1] P.D. Gujrati, Irreversibility, Molecular Chaos, and A Simple Proof of the Second Law, http://arxiv.org/abs/0803.1099 (arXiv:0803.1099) [2] P.D. Gujrati, Poincare Recurrence, Zermelo’s Second Law Paradox, and Probabilistic Origin in Statistical Mechanics, http://arxiv.org/abs/0803.0983 (arXiv:0803.0983)

C1.00260 Response of a simple dynamical network to stress or strain, NASRIN AFZAL, MICHEL PLEIMLING, Virginia Polytechnic Institute and State University — Motivated by a recent series of experiments that study the response of the cytoskeleton of living cells to mechanical forces, we study numerically a simple dynamical network where new links are formed and existing links are dissolved with probabilities that can depend on time. We thereby mimic mechanical stress and strain by protocols where we rapidly change the geometry of the network. Interestingly, the number of links in the network displays a nontrivial time dependence during these protocols.

C1.00261 Node weight distribution and disparity of some bipartite networks, XIU-LIAN XU, CHUN-HUA FU, DA-REN HE, College of Physics Science & Technology, Yangzhou University — We present an empirical investigation of 14 real world networks, which can be described by bipartite graphs. Each node is assigned a node weight, which denotes the obtained competition result. Firstly, empirically we observed that the total node weight distributions of all the systems may be fitted by shifted power law function form. The key parameters of the function can be used to describe the disparity. Secondly, a node weight disparity is defined for the same purpose. The empirical relationships between the parameters are obtained. The results show that the node weight distribution is very uneven. 

C1.00262 Properties of four real world collaboration-competition networks, CHUN-HUA FU, XIU-LIAN XU, DA-REN HE, College of Physics Science & Technology, Yangzhou University — Our research group has empirically investigated 9 real world collaboration networks and 25 real world cooperation-competition networks. Among the 34 real world systems, all the 9 real world collaboration networks and 6 real world cooperation-competition networks show the unimodal act-size distribution and the shifted power law distribution of degree and act-degree. We have proposed a collaboration network evolution model for an explanation of the rules [1]. The other 14 real world cooperation-competition networks show that the act-size distributions are not unimodal; instead, they take qualitatively the same shifted power law forms as the degree and act-degree distributions. The properties of four systems (the main land movie film network, Beijing restaurant network, 2004 Olympic network, and Taobao notebook computer sale network) are reported in detail as examples. Via a numerical simulation, we show that the new rule can still be explained by the above-mentioned model. [1] H. Chang, B. B. Su, et al. Physica A, 2007, 383: 687-702.

C1.00263 A model of the world languages distribution, AI-XIA FENG, DA-REN HE, College of Physics Science and Technology, Yangzhou University — The world language distribution is described by a bipartite graph. One kind of nodes is the languages; the other is the countries where some languages are used. When interested in interactions between the languages, we project the bipartite graph onto the language nodes and obtain a unipartite graph. After investigating the node strength distribution of the unipartite network we realize that the language distribution shows a kind of duality property. Thus, we set up a model to interpret and explain the property. Also, we explained, by using the model, the empirical results about the clustering coefficient distribution and the average nearest neighbor strength distribution.

C1.00264 Monte-Carlo simulations for two-stage percolation transition of the enhanced trees, TAKEHISA HASEGAWA, TOMOAKI NOGAWA, The University of Tokyo — We investigate the bond percolation problem on the enhanced binary tree (EBT). The EBT is given by adding intra-generation links to the binary tree. The EBT belongs to the class of nonamenable graphs (NAGs), and percolations on NAGs are predicted to show two-stage transition through three distinct phases according to open bond probability \( p \): (i) nonpercolating phase: there is no infinite cluster for \( 0 \leq p < p_{c1} \), (ii) intermediate phase: there are infinitely many infinite clusters for \( p_{c1} < p < p_{c2} \), and (iii) percolating phase: there is a unique infinite cluster for \( p_{c2} < p \leq 1 \). In this talk, we perform Monte-Carlo simulations to study the bond percolation on the EBT [1]. Our numerical results actually show that the system has two different percolation thresholds \( p_{c1} \) and \( p_{c2} \). By performing finite size scaling for the cluster size distributions, we confirm that all the points in the intermediate phase are critical. This fact leads to the existence of infinitely many infinite clusters in the intermediate phase. In this phase the corresponding fractal exponent continuously increases with \( p \) from zero to unity. We also show that the first transition at \( p_{c1} \) is of second order in mean field universality class, while order parameter rises discontinuously at \( p_{c2} \).

C1.00265 Interest rate change and Omori dynamics in the Stock Market, ALEXANDER PETERSEN, FENGZHONG WANG, Boston University, SHLOMO HAVLIN, Bar-Ilan University, H. EUGENE STANLEY, Boston University — I present the behavior of U.S. markets on the day of U.S. Federal Open Market Committee (FOMC) meetings from the perspective of Statistical Physics. The announcement of key U.S. Federal Reserve rate changes causes a small financial shock, where the dynamics before and after the announcement can be described by an Omori law. We find that markets respond sharply to news in a complex way reminiscent of physical earthquakes described by the Omori law, which describes the power-law relaxation of aftershocks following a singular perturbation. We find Omori laws in both the volatility of the price (also known as the absolute returns) and the volume traded, using 1-minute resolution financial time series. These results suggest that the perturbative response of the stock market is the same for both financial news and financial crises. The intraday response can be measured by the Omori power-law exponent \( \Omega \), which has opposite sign before and after the announcement. We estimate the magnitude of news by relating \( \Omega \) to the behavior of the U. S. Treasury Bill before and after FOMC announcements.

C1.00266 Structure of correlations with partially surrogated price fluctuations, GYUCHANG LIM, SOOYONG KIM, KAIST, KI-HO CHANG, KMA, KYUNGSIK KIM, Pukyong National university — The well-known facts of financial markets support that the price fluctuation contains information about the complexity of interactions among market participants. In this work, we present a new surrogate method to find the dependency of higher-order correlations on the magnitude of price fluctuations. By sorting returns into several groups with respect to the level of fluctuations, we show that the large fluctuations characterize the structure of temporal correlations of a financial time series. In particular, by investigating the positive and negative parts separately, we confirm that risk-averse behavior of traders is explicitly observed in financial markets.
C1.00267 Sediment transport dynamics of a river network in a long period\textsuperscript{1} \hfill JIE HUO, RUI HAO, XU-MING WANG, Physics and Electric Information Sciences, Ningxia University, Yinchuan 750021, P.R. China, COMPUTATIONAL & NONLINEAR PHYSICS STUDIO TEAM — A sediment transport model that connects a lower-water season to the higher-water season is suggested to study the dynamics in a long-term evolution process. The model is based on the feedback mechanism between sediment-carrying capacity of stream and erosion-deposition state of channels. It is checked by comparing the simulated results with the observed data of the Yellow River. The comparison can be conducted in two aspects. One is the comparison between the model results on every segment and the real results; the other is the estimation whether the variation trends of the calculated results are qualitatively in accordance with that occurred in the natural river network. The comparisons show that our model is reasonable. The detail of the dynamics manifests that the model can generate the general inherent characteristics of a real river network as it passes through a lower-water season to the higher-water season. This might provide us with a new visual angle for the researches in some related fields.

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C1.00268 Probing Localization in Scattering Systems via Fidelity \hfill MEI CHAI ZHENG, Dept. of Physics, JOSHUA BODIFELT, Dept. of Physics, Wesleyan University, ULRICH KUHL, HANS–JUERGEN STOECKMANN, Fachbereich Physik der Phillipus–Universität Marburg, TSAMIKOS KOTTOOS, Max Planck Institute for Dynamics & Self-Organization. AND Dept. of Physics, Wesleyan University, DEPT. OF PHYSICS, WESLEYAN UNIVERSITY COLLABORATION, FACHBEREICH PHYSIK DER PHILLIPS–UNIVERSITÄT MARBURG COLLABORATION, MAX PLANCK INSTITUTE FOR DYNAMICS & SELF-ORGANIZATION COLLABORATION — Using scattering measurements from a microwave cavity filled with randomly distributed scatterers, we evaluate the scattering fidelity. We show that depending on the degree of localization inside the sample, the fidelity decay deviates from “traditional” Gaussian law, applied in the case of diffusive/chaotic cavities when small perturbations are involved. We instead show that for small displacements of one of the walls of the cavity, the fidelity decays in a novel way that reflects the degree of localization (or randomness) inside the cavity. The outcome of the experimental measurements are explained on the basis of a parametric Banded Random Matrix modeling which incorporates localization phenomena. The theoretical results are in good agreement with those of the experiment.

C1.00269 Experimental observation of soliton propagation and annihilation in a hydromechanical array of one-way coupled oscillators \hfill PATRICK M. ODENTHAL, JOHN F. LINDNER, KELLY M. PATTON, JAMES C. GALLAGHER, Department of Physics, The College of Wooster, Wooster OH 44691, BARBARA J. BREEN, Department of Physics, University of Portland, Portland OR 97203 — We have experimentally realized unidirectional or one-way coupling in a mechanical array by powering the coupling with flowing water. In cyclic arrays with an even number of elements, soliton-like waves spontaneously form but eventually annihilate in pairs, leaving a spatially alternating static attractor. In cyclic arrays with an odd number of elements, this alternating attractor is topologically impossible, and a single soliton always remains to propagate indefinitely. Our experiments with 14 and 15-element arrays highlight the dynamical importance of both noise and disorder and are further elucidated by our computer simulations. This work was supported in part by NSF DMR-0649112.

C1.00270 Order and Chaos in the Two-Body Problem \hfill JACOB LYNN, FRANK W. KING, JOHN F. LINDNER, Department of Physics, The College of Wooster, Wooster OH 44691 — We investigate a simple extension of the classical two-body problem involving the gravitational interaction of a point and a line segment. We find families of periodic orbits amidst chaotic orbits in both the parameter and initial condition spaces. We characterize the dynamics using animations, Poincare sections, distance metrics, power spectral densities, and Lyapunov exponents. This work was supported in part by NSF DMR-0649112.

C1.00271 Simulation of the Dynamics of a Plane Pendulum with Positional Dependent Torque\textsuperscript{1} \hfill TODD MCALPINE, Ohio Northern University, ALISON HUFF, The College of Wooster — We investigate the dynamics of a plane pendulum with positional dependent driving torque as would be produced by a horizontally directed force exerted on the pendulum bob. We compare and contrast this with the well known solutions of the classical pendulum. In cyclic arrays with an even number of elements, soliton-like waves spontaneously form but eventually annihilate in pairs, leaving a spatially alternating static attractor. In cyclic arrays with an odd number of elements, this alternating attractor is topologically impossible, and a single soliton always remains to propagate indefinitely. Our experiments with 14 and 15-element arrays highlight the dynamical importance of both noise and disorder and are further elucidated by our computer simulations. This work was supported in part by NSF DMR-0649112 and The College of Wooster for their support.

C1.00272 SUPERCONDUCTIVITY —

C1.00273 A Systematic Photoemission Study of the Fe(Te\textsubscript{1-x}Se\textsubscript{x}) Superconductor System \hfill YUOUI XIA, Princeton University, N. L. WANG, Institute of Physics, Chinese Academy of Science. ZAHID HASAN, Princeton University — We present a systematic photoemission study of the newly discovered superconducting class Fe(Te\textsubscript{1-x}Se\textsubscript{x}). By using a series of photon energies and scattering geometries we investigated the details of the quasiparticle dispersion, Fermi surface and the global band structure. Doping dependent phase diagram study into the superconducting regime would be reported.

C1.00274 High energy anomaly in hole- and electron-doped cuprates \hfill B. MORITZ, SLAC and Stanford University, F. SCHMITT, W. MEEVASANA. Stanford University, S. JOHNSTON, University of Waterloo, E. M. MOTOYAMA, M. GREVEN, Stanford University, D. H. LU, SLAC, C. KIM, Yonsei University, R. T. SCALETAR, University of California-Davis, Z.-X. SHEN, T. P. DEVEREAUX, SLAC and Stanford University — Recent ARPES experiments reveal the presence of a dispersion anomaly in the high T\textsubscript{c} cuprates. This universal anomaly appears at an energy of \( \sim 300 \) meV in hole-doped compounds, with a similar feature reported in the half-filled parent insulators. New experiments on Nd\textsubscript{2-x}Ce\textsubscript{x}CuO\textsubscript{4} also reveal an anomaly, but at a higher energy scale of \( \sim 500 - 600 \) meV. A key question concerns the origin of this anomaly. Quantum Monte Carlo simulations of the single-band Hubbard model reveal qualitative and quantitative agreement with the dispersion anomaly throughout the doping spectrum. They demonstrate that strong correlations play a key role in the development of the anomaly as well as that of spectral weight transfers that accompany doping.

C1.00275 Determination of the Eliashberg's Equations in the Superconductivity Post BCS \hfill CARLOS FIGUEROA, RENE BETANCOURT, LAZARO FERRER, MARTIN MOLINAR, DIFUS — The Eliashberg theory was a significant advance with respect to the BCS Theory because of it extends the rank of application without changing its origin, which is based on the formation of Cooper pairs by the interaction electron phonon. It doesn’t modify the essential characteristics of BCS theory but it includes more information about the subject. Another point to be considered is BCS theory works, better with the weak electron-phonon coupling superconductors as the aluminium (Al). As the coupling becomes strong the results show significant deviations as in the case of lead (Pb). The Eliashberg’s equations make an extension to incorporate the strong electron-phonon interaction. This theory synthesizes the information in a expression known as Eliashberg’s function, or effective spectral density. Using the last problem solutions it can be possible to recover the universal relation of the BCS, likewise, the deviation function and the isotope effect. No doubt, it is a qualitative jump in the knowledge of the conventional superconductor materials.
C1.00276 Condensation of topological excitations in two coupled layers of Josephson junction arrays. SAID SAKHI, American University of Sharjah, PO Box 26666, Sharjah, UAE. The phase diagram of two coupled layers of Josephson junction arrays (JJAs) in the presence of charge and magnetic frustration is investigated. The quantum phase model of JJAs is mapped into the self-dual limit into an Abelian gauge theory with Maxwell terms and a mixed Chern–Simons term. The low effective field theory is shown to be governed by complex fields associated with disordering caused by electric charges and magnetic charges minimally coupled to two gauge fields related to the currents of Cooper pairs and vortices. The condensation of disorder fields leads to a rich phase diagram with important features not attainable by standard mean field theories. In addition to insulating and superconducting phases, the bi-layer system displays interesting interplay between Hall quantization and interlayer coherence. Hall quantized states with and without interlayer coherence and interlayer coherent states without Hall quantization. S. Sakhi, Quantum disordering effects in bilayer Josephson junction arrays, J. Phys. A: Math. Theor. 41 (2008) 085003.

C1.00277 The Electronegativity Spectrum of Superconductors. O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies, Abuja FCT. In the experimental search for novel superconductors, the correlation of electronegativity with superconductivity has been a useful guide. Previous studies have identified the range of electronegativities for low and high Tc superconductors. A detailed spectrum plot of electronegativity versus transition temperature for all known superconductors has still not been published. Here we produce such a plot which includes electronegativities of the newly discovered iron-based pnictide superconductors. We analyze this spectrum plot and use it to predict the electronegativity of higher Tc superconductors.

C1.00278 Experimental and Theoretical Investigation of High Temperature Superconductors. SCOTT DIETRICH, Boston University. The study includes ongoing physical measurements on High Temperature Superconducting (HTS) samples. A dual-coil apparatus, using BSCCO and YBCO samples, is used to measure the magnetic susceptibility, resistivity and other measurements of the samples. This allows for the inspection of the HTS material during its superconducting state, above the critical temperature and the region in between. Using this data, we hope to model the HTS material using a mathematically driven computer simulation. The simulation models the material as a matrix of Josephson Junctions and can apply the variables added into the lab, including electrical current, magnetic field, and temperature variation. The simulation aims at explaining the mechanisms behind high temperature superconductivity. Included in the program is the option to change lattice structures, giving the ability to explore theoretical HTS material compositions and preview their actions compared to the commonplace square lattice structures.

C1.00279 Force analysis of a permanent magnet and a superconducting hollow cylinder. MOHAMMED ALQADI, The interaction between a cylindrical magnet and a superconducting hollow cylinder in the Meissner state was analyzed using dipole-dipole model. Analytical expression of the levitation force was derived as a function of the magnetic moment, radius of the magnet, radius and thickness of the superconductor sample. The obtained results show that there is strong dependence of the levitation force on the magnetic dipole orientation at a small magnet-superconductor distance.

C1.00280 C-axis persistent current and Cooper-pair tunnelling through intrinsic Josephson junctions in a ring-shaped YBa2Cu3O7−δ film. AHMAD MANSOUR, MOHAMED SABER, KIM CHOW, JAN JUNG, University of Alberta. We present the direct experimental observation of the temperature dependence of the persistent current Ic due to tunneling Cooper pairs along the c-axis intrinsic Josephson junctions integrated into YBa2Cu3O7−δ ring-shaped thin films. The measured Ic exhibits a linear temperature dependence over a wide range of temperatures well below Tc. Similar behavior was observed in different samples, confirming the reproducibility of the fabrication technique and the reliability of the results. Our fabrication and measurement techniques which allowed us to observe “pure” Cooper pair tunneling persistent current are superior to other techniques that are unable to separate Cooper pair from quasi-particles tunneling currents.

C1.00281 Probing KT transition using ac current. HENGSONG ZHANG, The state university of New York Buffalo. FULIN ZUO, University of Miami. We report studies of the Kosterlitz-Thouless (KT) transition in thin thin films using an ac excitation current rather than the conventional dc current. The nonlinear dependence or power-law exponent of the voltage on current is probed by measuring the harmonic terms of the voltage signal. The voltage can in general be expressed as a sum of odd-powered current terms with the experimentally measured power exponent increasing with lowering temperature. The temperature and current dependence of the exponent have been studied and will be discussed in terms of vortex-antivortex pair and pair-pair interactions.

C1.00282 Phase Separated Bose-Einstein Condensate for High Sensitivity Force Measurement. SATYAN BHONGALE, Rice University. EDDY TIMMERMANS, Los Alamos National Laboratory. A trapped, phase separated, two component Bose-Einstein condensate (BEC) can be configured to give a single BEC bubble that floats freely in the surrounding BEC. We point out that this system gives a unique template to carry out mesoscopic quantum studies and to detect weak forces. We demonstrate the detection capabilities by proposing and studying a “Quantum Level” for fundamental quantum fluctuation studies and for mapping the potential energy landscape near a surface with exquisite accuracy. We show that for typical (modest) values of currently available experimental parameters, the proposed device is sensitive to the variations in gravitational acceleration to 1 part in 10 billion. While such sensitivity is in the range of other available devices, for example torsion balance, the BEC device allows for measuring the gravitational acceleration on length scales of the order of a few microns.

C1.00283 Definition of current density in presence of AC electric field. ZHANG LEI, WANG JIAN, Department of Physics, University of Hong Kong. Under time varying AC electric field, the transport problem becomes complicated due to the presence of displacement current. The conventional current density calculated by using the formula \( J_r = \frac{1}{2\pi c} \text{Re} \left( \frac{\psi}{(p-eA)} e^\Omega - \text{c.c.} \right) \) is not conserved, which means \( \nabla \cdot J_r (r,t) \neq 0 \). In order to solve this problem, we will give a new definition of current density by using non-equilibrium Green’s function which includes the contributions from the Coulomb interaction in low frequency limit. And we will show that the current calculated from the current density is conserved.

1Research support from Mr. Ferguson Uzoma, PhD Bank, Abuja FCT, Nigeria and ISEM, University of Wollongong, New South Wales 2522, Australia.

2Mentor: George Zimmermann
C1.00284 The dynamic critical exponent in optimally doped Pr$_{1.85}$Ce$_{0.15}$CuO$_4$ as a function of film inhomogeneity$^1$, R.A. ISAACS, J. B. OLSON, J. SOUSA, M. SALVAGGIO, M.C. SULLIVAN, Department of Physics, Ithaca College, Ithaca NY, R.L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland College Park — Scaling analysis of voltage vs. current isotherms is a good tool to study the normal-superconducting phase transition in cuprate conductors. This measurement has never been performed on the optimally doped cuprate conductor Pr$_{1.85}$Ce$_{0.15}$CuO$_4$. If we take the finite thickness of the films into account$^{[2]}$ we can find the critical isotherm and determine the dynamic critical exponent $z$ in our Pr$_{1.85}$Ce$_{0.15}$CuO$_4$ films. We find that the critical exponent varies as a function of transition width, from which we can infer the effect of sample inhomogeneity on the dynamic critical exponent. We present our results of the critical exponent as a function of sample inhomogeneity and compare it to the hole-doped cuprate YBa$_2$Cu$_3$O$_7$.$\delta$.

$^1$Supported by NSF grant DMR-0706557


C1.00285 A study of the critical current density in optimally-doped, thin-film cuprate superconductor YBa$_2$Cu$_3$O$_7$.$\delta$$^1$, E.S. BACKUS, M. LILLY, M.C. SULLIVAN, Department of Physics, Ithaca College, Ithaca, NY — Scaling analysis of voltage vs. current isotherms has often been used to study the normal-superconducting phase transition in cuprate superconductors, though there is little consensus in the literature as to the values of the critical exponents for this phase transition. Studying the critical current will give us another way to examine the normal-superconducting phase transition, and perhaps rectify the lack of consensus regarding the critical exponents. We designed a photolithographic mask with several meander patterns to test, varying the lengths and thicknesses of the patterned wires. We conducted reverse-polarity measurements sent through the meander patterns of thin-films of the cuprate superconductor YBa$_2$Cu$_3$O$_7$.$\delta$. Because the critical current density in this material is so high, several extrinsic effects must be taken into consideration in order to avoid heating, including: determining the most effective number of measurements, the wait time between measurements, and the wait time between increments of temperature in order to reduce the error. I present my results as a plot of the critical current as a function of temperature in zero-field, and the critical exponent.

$^1$Supported by NSF grant DMR-0706557.

C1.00286 Influence of diffusion-annealing time on the mechanical properties of bulk Bi$_{1-x}$Pb$_x$Sr$_{1-y}$Ca$_2$Cu$_3$O$_{y+2}$ superconductors diffusion-doped with Fe.$^1$, MUSTAFA AKDOGAN, Abant Izzet Baysal University, OZGUR OZTURK, Kastamonu University, ERSIN YUCEL, ERDAL BEKIROGLU, Abant Izzet Baysal University, MUSTAFA YILMAZLAR, Sakarya University, CABIR TERZIOGLU, Abant Izzet Baysal University — In order to investigate the role of Fe doping and diffusion-annealing duration on the mechanical and superconducting properties of Bi-Pb-Sr-Ca-Cu-O, Bi$_{1-x}$Pb$_x$Sr$_{1-y}$Ca$_2$Cu$_3$O$_{y+2}$ superconductors were prepared by standard solid-state reaction methods. Doping of Bi-2223 was carried out by means of iron diffusion during sintering from an evaporated iron film on pellets. The investigations consist of SEM, dc resistivity and hardness measurements. These measurements indicated that the Fe doping and diffusion-annealing time increased the $T_c$, $J_c$, Young’s modulus(E), yield strength(Y), fracture toughness(K$_IC$) values and improved the grain connectivity. The mechanical properties of the samples were found to be load dependent and on the diffusion-annealing time. In addition, we calculated the load independent $H_0$, E, Y, and K$_IC$ of the samples. Possible reasons for the observed improvements in the superconducting and mechanical properties due to Fe diffusion are discussed.

$^1$This work supported by TUBITAK under grant contract No: 104T323 and 104T325

C1.00287 Soft X-ray Imaging of Vortex Dynamics in Trilayer Pattered Magnetic Elements, BROOKE MESLER, Applied Science and Technology Graduate Group, University of California at Berkeley, DONG-HYUN KIM, Dept of Physics, Chungbuk National University, Kumpa, PETER FISCHER, Center for X-ray Optics, Lawrence Berkeley National Lab — Soft X-ray microscopy provides element specific magnetic imaging with a spatial resolution down to 15nm. At XM-1, the full-field soft X-ray microscope at the Advanced Light Source in Berkeley, a stroboscopic pump and probe setup has been developed to study fast magnetization dynamics in ferromagnetic elements with a time resolution of 70ps which is set by the width of the X-ray pulses from the synchrotron. Previous studies of patterned permalloy elements have revealed complex magnetization dynamics. Results obtained with a 2um x 4um x 45nm rectangular permalloy sample exhibiting a seven domain Landau pattern reveal dynamics up to several nsec after the exciting magnetic field pulse. Domain wall motion, a gyrotropic vortex motion, and a coupling between vortices in the rectangular geometry are observed. On going studies of patterned trilayer elements, composed of magnetic permalloy and cobalt layers separated by a copper spacer layer, will probe the dynamics of the trilayer system. Of particular interest is observing how the coupling between the magnetic layers affects the vortex dynamics.

C1.00288 Two dimensional magnetization mapping in exchange-coupled nanodot chain arrays using the magneto-optic Kerr effect, SARAH C. HERNANDEZ, JIAN DOU, CHENGTAO YU, MICHAEL J. PECCHAN, Department of Physics, Miami University, LIESL FOLKS, JORDAN A. KATINE, MATTHEW J. CAREY, San Jose Research Center, Hitachi Global Storage Technologies — Nanoscale permalloy dot arrays were fabricated with dot diameters of 300 nm, thicknesses of 40 nm, and coupled via permalloy bridges, with bridge widths ranging from zero to 60 nm. Magnetization reversal in this system was previously investigated with the field applied along and perpendicular to the coupling direction. Hysteresis loops reflect reversal by domain wall motion$^1$. As a result of rotating the applied magnetic field relative to the sample’s coupling direction, unusual hysteresis loops were observed. The magneto-optic response resulted in an asymmetric loop with one notable feature, an increase in coercivity with increasing bridge width. We will show that these curves arise from the second-order magneto-optic Kerr effect, where coherent rotation of magnetization plays an important role. This work is supported by US-Dept.of Energy at MU.

$^1$S. C. Hernandez et al, (To be published in J. Appl. Phys.)

C1.00289 Superconducting properties of tetragonal FeSe and FeTe, YOSHIAKAZU MIZUGUCHI, YOSHIHIKO TAKANO, NIMS — The discovery of LaFeAsO1-xFx superconductor triggered active studies on iron-based superconductors. Recently, superconductivity in tetragonal FeSe was reported. FeSe is the simplest-structured iron-based superconductor. We reported a huge enhancement of the transition temperature $T_c$ under high pressure. The onset of $T_c$ increased from 13 to 27 K at 1.48 GPa. FeSe undergoes a structural phase transition to orthorhombic around 70 K. A suppression of the structural phase transition will be a key to raise $T_c$ in this system. Tetragonal FeTe has a structure very analogous to that of superconducting FeSe, however, does not show superconductivity, and undergoes a structural phase transition around 80 K. We synthesized S-substituted FeTe, FeTe1-$x$Sx, and observed the suppression of the structural phase transition and superconductivity at low temperatures. Since FeTe1-$x$Sx is composed of nontoxic elements, this compound is advantageous for applications. Here we report the pressure and the elementary substitution effects on FeSe, the pressure studies on FeTe, and the superconducting properties of FeTe1-$x$Sx.
C1.00290 Effects of sintering temperature on properties of Ti-sheathed, SiC-doped MgB2 superconducting wires, GAN LIANG, HUI FANG, Sam Houston State University, CAD HOYT, Cornell University, SAMARESH GUHHAIT, JOHN MARKERT, University of Texas at Austin — Mono-core Ti-sheathed, silicon carbide (SiC) doped MgB2 wires have been successfully fabricated by powder-in-tube method. The average size of the doped SiC nano particles is 20 nm and the doping level is 10 wt.%. The wires were sintered for 30 minutes at five temperatures from 650 °C to 800 °C. Effects of sintering temperature on the phase composition, microstructure, and critical current density (Jc) were studied by x-ray diffraction, scanning electron microscopy, and magnetization measurements. The results indicate that the Ti sheath does not react with the magnesium and boron, and the present wire rolling process can produce Ti-sheathed, SiC-doped MgB2 wires with high critical current density. It is found that Jc peaks up at sintering temperature of 800 °C. This is in sharp contrast with the previously reported result (by other group) that the optimal Jc was achieved at sintering temperature of 700 °C. The correlations between Jc and the structural properties of the wires are discussed.

C1.00291 Meissner effect in ensemble of slightly boron-doped carbon nanotubes, J. HARUYAMA, N. MURATA, Aoyama Gakuin Univ., J. REPPERT, A. RAO, Clemson Univ., T. KORETSUNE, S. SAITO, Tokyo Institute of Technology — The small mass of carbon can promote high transition temperature (Tc) in BCS-type superconductivity (SC). Recently, new carbon-based superconductors with order of Tc of ~10K [1, 2] were discovered and higher Tc has been expected. In particular, the SC in a carbon nanotube (CNT) is attracting considerable attention [3]. We reported that entirely end-bonded multi-walled CNTs, in which Luttinger liquid was suppressed, could show SC with Tc = 12K, previously [4]. In contrast, it had problem in reproducibility, because correlation with carrier doping was not clarified. Moreover, none has succeeded substitutional carrier doping into CNTs and also revealed the correlation with SC. Here, we report on the Meissner effect with Tc =12K found in thin films consisting of boron-doped single-walled CNTs [5]. We reveal that boron concentration < 1.5 at.% in the CNTs and those highly homogeneous assembling to thin films are favorable to yield evident Meissner effect. This can be understood by better adjustment of Ef to van Hove singularity in density of states. [1] T. E. Weller et al., Nature Physics 1, 39 (2005), [2] E. A. Ekimov et al., Nature 428, 542 (2004), [3] M. Kociak et al., Phys. Rev. Lett. 86, 2416 (2001), [4] I. Takesue, J. Haruyama, et al., Phys. Rev. Lett. 96, 057001(2006), [5] N. Murata, J. Haruyama, et al., Phys.Rev.Lett. 101, 020702 (2008)

C1.00292 Coexistence between magnetism and superconductivity in the HgMn0.3Pb2 compound, AUDUSIN DANILO BORTOLOZO, Escola de Engenharia de Lorena - EEL - USP-Brazil, ERIKA CARLINA A. SANTANA, Faculdade de Engenharia de Guaratinguetá - FEG - Brazil, CARLOS ALBERTO M. DOS SANTOS, ANTONIO JEFFERSON S. MACHADO, Escola de Engenharia de Lorena - EEL - USP-Brazil — In this work we will show the influence Mn doping in the HgPb phase. The HgMn0.3Pb2 phase is investigated by x-ray diffraction, magnetic and electrical resistivity measurements. Polycrystalline samples with HgMn0.3Pb2 nominal compositions were prepared by solid state reaction. X-ray powder diffractograms suggest that all peaks can be indexed with the tetragonal phase of AuCu prototype. The R(T) data for the HgMn1−xPb2 composition reveals superconductor behavior below 5.9K. The careful analysis of M(T) data reveals magnetic ordering close to 45K with saturation around the superconducting transition. The Mn doping in the HgPb2 phase suggests the magnetic ordering it is occurring in the specific plane occupied by Mn atoms. The M(H) show typical type-II superconductor which we estimate the Hc1 approximately 240 Oe. This work, report by first time the coexistence between magnetism and superconductivity in an AuCu prototype compound

C1.00293 Designing Superconductors with Periodic Table-based Maps and Material Databases1, O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies, Abuja FCT, ALEX ANIMALU, Department of Physics and Astronomy, University of Nigeria, Nsukka — One of the grand challenges of superconductivity science is achieving a paradigm shift from discovery by serendipity to discovery by design. Empirical and heuristic rules have been a useful bridge in this desired direction. Many early superconductors were discovered by this method and by serendipity. DFT-based ab initio methods have often ignored empirical and experimental data. Here we propose that by using Periodic Table-based maps such as electronegativity spectrum maps, valence electron spectrum maps and atomic number spectrum maps for binary systems, A,Bx, combined with data-mining of experimental material databases we can “reverse-engineer” many known superconductors. We demonstrate the power of this technique by predicting new and novel superconductors without recourse to DFT calculations.

1 Research support from Dr. Michael Schaffer, General Atomic, San Diego, CA.

C1.00294 Microscopic transport in indium oxide thin films near the superconductor-insulator quantum phase transition, MINSOO KIM, TAILUNG WU, ZHENZHONG SHI, ADAM STABILE, G. SAMBANDAMURTHY, University at Buffalo-SUNY, Buffalo, NY 14260 — We present results from low temperature (T), MINSOO KIM, TAILUNG WU, ZHENZHONG SHI, ADAM STABILE, G. SAMBANDAMURTHY, University at Buffalo-SUNY, Buffalo, NY 14260 — We present results from low temperature (T), high magnetic field (B) transport measurements on disordered thin films of amorphous indium oxide. Two-dimensional (2D) indium oxide films can be driven between insulating and superconducting ground states by controlled tuning of either the intrinsic disorder or external B. We have grown these films with hitherto unachieved control of their structure and property and patterned into Hall bars and nanowires using standard nanolithographic techniques for transport measurements. Here we present the results of a study of the resistance behavior in these films in the 1D and also in the 1D-2D crossover regimes when the ground state in the T = 0 limit is tuned from an insulator to a superconductor. Our efforts are aimed at achieving, for the first time, a continuously tunable 1D superconductor.

C1.00295 The Superconducting Transition in Al Nanowires, PAUL ALIOTTA, JOHN FREE, Harvard University and Eastern Nazarene College, ROBERT WESTERVLET, Harvard University — Strong evidence for macroscopic quantum tunneling has been presented in Al wires with diameters less than 10 nm [1], which is much lower than the material’s coherence length. We have investigated the superconducting transition and evidence for macroscopic quantum tunneling in Al nanowires with diameters ranging from 10 to 40nm. We will present data for these wires.


C1.00296 Pressure effects on superconductivity and magnetism in FeSe0.88 and FeSe1−xTe x, CHIEN-LUNG HUANG, CHI-CHIE CHOU, KOU-FENG TSENG, YI-LIN HUANG, FONG-CHI HSU, KUO-WEI YEH, HUNG-DUEN YANG, National Sun Yat-sen University — We have performed the pressure (P) dependence of ac, dc susceptibility and resistivity measurements on iron chalcogenides FeSe0.88, FeSe0.5Te0.5, FeSe and FeTe0.05. The superconducting transition temperature (Tc) of FeSe0.88 is found to increase with P linearly at a rate of dTc/dP ∼ 3.09×10−2 K/kbar, while the Tc of FeSe0.5Te0.5 increases nonlinearly with an initial rate of 1.47K/kbar then saturates at P ∼ 18 kbar. Such the enhancement of Tc might be attributed to an increase of density of states. There is no indication of superconductivity observed in FeTe and FeTe0.9, which is inconsistent with the result of theoretical calculation, and it might be due to the existence of long range magnetic spin coupling that inhibits the formation of superconductivity mediated by spin fluctuations, which is applied to describe the mechanism in Fe-based superconductors.

C1.00297 ABSTRACT HAS BEEN MOVED TO S1.00263 —
C1.00298 Superconductivity in (La, Y)FeAs(O, F) pnictides, MATTEO TROPEANO, LAMIA-INFM-CNR, Genova-Italy & Dipartimento di Fisica, Genova-Italy, CARLO FERDEGHINI, LAMIA-INFM-CNR, Genova-Italy, CARLO FANCIULLI, LAMIA-INFM-CNR, Genova-Italy, ALBERTO MARTINELLI, LAMIA-INFM-CNR, Genova-Italy, ANDREA PALENZONA, Dipartimento di Chimica e Chimica Industriale, Genova-Italy & LAMIA-INFM-CNR, MARINA PUTTI, LAMIA-INFM-CNR & Dipartimento di Fisica & Applied Superconductivity Cen, ROBERTA CIMBERLE, IMEM-CNR, Genova-Italy, FABIO CANEPA, Dipartimento di Chimica e Chimica Industriale, Via Dodecaneso 31, 16146 Genova ITALY & IMEM-CNR, Genova-Italy — The structural, magnetic and resistive properties of (La, Y)FeAs(O, F) compounds prepared at normal pressure were investigated. Substituting La with Y decreases the ionic size at the rare earth site, determining a progressive decrease of both cell edges; as a result a notable increase of the superconductive transition temperature is observed. In particular Tc increases with Y content, up to a maximum value of 39.8 K for x = 0.5, followed by the a slight decrease for x = 0.7 (Tc = 35.9 K). The resistivity curve of the corresponding undoped compound, (La0.5Y0.5)FeAsO, exhibits the typical bump related to the SDW onset; the first derivative curves for (La0.5Y0.5)FeAsO and LaFeAsO are almost superposed around TSDW.

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D1 DCMP: Phase Transitions and Transport in Quantum Hall Superfluids

2:30PM D1.00001 Phase Diagram of Bilayer 2D ElectronSystems at \( \nu_T = 1 \), ALEXANDRE CHAMPAGNE, Caltech — Bilayer 2D electron systems at total filling fraction \( \nu_T = 1 \) and small interlayer spacing can support a strongly correlated phase which exhibits spontaneous interlayer phase coherence and may be described as an excitonic Bose condensate. We use electron interlayer tunnelling and transport to explore the phase diagram of bilayer 2D electron systems at \( \nu_T = 1 \), and find that phase transitions between the excitonic \( \nu_T = 1 \) phase and bilayer states which lack significant interlayer correlations occur in three different ways: by increasing the effective interlayer spacing, \( d/\ell \), the temperature, \( T \), or the charge imbalance, \( \Delta \nu = \nu_1 - \nu_2 \). First, for the balanced (\( \Delta \nu = 0 \)) system we find that the amplitude of the resonant tunneling in the coherent \( \nu_T = 1 \) phase obeys an empirical power law scaling versus \( d/\ell \) at various \( T \), and the layer separation where the tunneling disappears scales linearly with \( T \). Our results [1] offer strong evidence that a finite temperature phase transition separates the balanced interlayer coherent phase from incoherent phases which lack strong interlayer correlations. Secondly, we observe [2] that close to the phase boundary the coherent \( \nu_T = 1 \) phase can be absent at \( \Delta \nu = 0 \), present at intermediate \( \Delta \nu \), and absent again at large \( \Delta \nu \), thus indicating an intricate phase competition between it and incoherent quasi-independent layer states. Lastly, at \( \Delta \nu = 1/3 \) we report [2] the observation of a direct phase transition between the coherent \( \nu_T = 1 \) bilayer integer quantum Hall phase and the pair of single layer fractional quantized Hall states at \( \nu_1 = 2/3 \) and \( \nu_2 = 1/3 \).


3:06PM D1.00002 \( \nu = 1/2 + 1/2 \) Quantum Hall Bilayers, STEVEN H. SIMON, Peierls Centre for Theoretical Physics, Oxford University — Quantum Hall bilayer systems at filling fractions near \( \nu = 1/2 + 1/2 \) undergo a transition from a compressible phase with strong intralayer correlation to an incompressible phase with strong interlayer correlations as the layer separation \( d \) is reduced below some critical value. Deep in the intralayer phase (large separation) the system can be interpreted as a fluid of composite fermions (CFs), whereas deep in the interlayer phase (small separation) the system can be interpreted as a fluid of composite bosons (CBs). The focus of this paper is to understand the states that occur for intermediate layer separation by using trial variational wavefunctions. We consider two main classes of wavefunctions. In the first class, previously introduced in [1], we consider interlayer BCS pairing of two independent CF liquids. We find that these wavefunctions are exceedingly good for \( d \approx d_0 \) with \( d_0 \) the magnetic length. The second class of wavefunctions naturally follows the reasoning of [2] and generalizes the idea of pairing wavefunctions by allowing the CFs also to be replaced continuously by CBs. This generalization allows us to construct exceedingly good wavefunctions for interlayer spacings of \( d \approx d_0 \) as well. The accuracy of the wavefunctions discussed in this work, compared with exact diagonalization, approaches that of the celebrated Laughlin wavefunction. More details can be found online in [3].


3:42PM D1.00003 Optical probes of excitonic phases in quantum Hall bilayers at \( \nu_T = 1 \), VITTORIO PELLEGRINI, NEST and Scuola Normale Superiore, Pisa (Italy) — In this talk we discuss our recent inelastic light scattering results that shed light on the interplay between incompressible and compressible quantum phases of electron bilayers at total filling factor \( \nu_T = 1 \). In the regime of finite values of tunneling gaps, we observe a quantum phase transformation between composite fermion (CF) metal and incompressible excitonic states as the tunneling gap is reduced. We show that the transition becomes discontinuous (first-order) by impacts of different terms of the electron-electron interactions that prevail on weak residual disorder [1]. The evidence is based on precise determinations of the excitonic order parameter and of measurements of CF spin excitations by resonant inelastic light scattering close to the phase boundary [2,3]. While there is marked softening of low-lying excitations, our experiments underpin the roles of competing order parameters linked to quasi-particle correlations in removing the divergence of quantum fluctuations [4]. In the regime of vanishingly small tunneling gaps we show that the abrupt disappearing of CF spin excitations below the spin-wave mode indicates the emergence of the inter-layer correlated quantum Hall state in the vicinity of \( \nu_T = 1 \) and when the temperature is lowered below a critical value [5]. Finally, the evolution of the spin-wave mode as a function of the Zeeman energy suggests the occurrence of a spin transition [5]. * Work done in collaboration with: B. Karmakar, A. Pinczuk, L. N. Pfeiffer, K. W. West.


4:18PM D1.00004 Theory of Activated Transport in Bilayer Quantum Hall Systems, H.A. FERTIG, Indiana University — We analyze the transport properties of bilayer quantum Hall systems at total filling factor \( \nu_T = 1 \) in drag geometries as a function of interlayer bias, in the limit where the disorder is sufficiently strong to unbind meron-antimeron pairs, the charged topological defects of the system. We compute the typical energy barrier for these objects to cross incompressible regions within the disordered system using a Hartree-Fock approach, and show how this leads to multiple activation energies when the system is biased. We then demonstrate using a bosonic Chern-Simons theory that in drag geometries, current in a single layer directly leads to forces on only two of the four types of merons, inducing dissipation only in the drive layer. Dissipation in the drag layer results from interactions among the merons, resulting in very different temperature dependences for the drag and drive layers. Connections with recent experiments will be discussed.

* This work was performed in collaboration with Bahman Roostaei, Kieran Mullen, and Steve Simon. Authors acknowledge support of the NSF.
Spin-dependent phase diagram in bilayer 2D electron systems, KOJI MURAKI, NTT Basic Research Laboratories — Bilayer electron systems with total filling \( \nu = 1 \) involve rich physics arising from the interplay between the intralayer and interlayer interactions parameterized by the ratio between the interlayer distance \( d \) and the magnetic length \( \ell_B \). One key issue in this system is the nature of the phase transition that occurs when exploring the system between the two limits of weak and strong interlayer interactions, i.e., compressible Fermi-liquid states of composite fermions and an incompressible quantum Hall state. Here we report tilted-field experiments on a double quantum well with negligible tunneling that demonstrate that the spin degree of freedom plays a decisive role in the ground-state phase diagram of this system [1]. When the ratio \( \eta \) of the Zeeman to Coulomb energies is enhanced by tilting the sample in a field by an angle \( \theta \), we observe that the phase boundary located at \( d/\ell_B = 1.90 \) for \( \theta = 0 \) shifts to higher densities until it saturates at \( d/\ell_B = 2.33 \) for \( \theta \geq 60 \) degree. The data thus establish a spin-dependent phase diagram as a function of \( \eta \) and \( d/\ell_B \). We model the energies of the competing phases treating the compressible state as nearly independent Fermi liquids of composite fermions. The excellent agreement between the model and experiment indicates that at small \( \theta \) the compressible state is only partially polarized and its Zeeman-dependent energy is responsible for the observed shift of the phase boundary, with the saturation at large \( \theta \) signaling the full polarization. This in turn implies that the intrinsic transition, expected for the ideal system without spin and intensively studied in theory, is preempted by a transition to a partially polarized compressible state in the standard experimental conditions and can only be revealed by suppressing the spin degree of freedom. Our results thus shed new light on previous experiments and show a way to investigate the intrinsic properties of the system. [1] P. Giudici et al., Phys. Rev. Lett. 100, 106803 (2008).

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D2 DCMP: HTSC: New Developments Spirit of Pittsburgh Ballroom BC

2:30PM D2.00001 New magnetic neutron scattering results for the high-Tc superconductors HgBa2CuO4+x and Nd2−xCexCuO4+y, MARTIN GREVEN, Stanford University — We have succeeded in growing sizable single crystals of HgBa2CuO4+x, the single-layer hole-doped compound with the highest superconducting transition temperature [1]. Careful characterization demonstrates the high quality of our crystals [2]. Using polarized neutron diffraction, we find an unusual magnetic order in the pseudogap phase [3]. Together with prior results for YBa2Cu3O6+δ, this observation constitutes a demonstration of the universal existence of such a state. Our inelastic neutron scattering measurements reveal that the antiferromagnetic resonance occurs at a rather high energy in HgBa2CuO4+x and, hence, that the resonance energy is not universally related to \( T_c \) [4]. Finally, our results for the antiferromagnetic excitations in Nd2−xCexCuO4+y provide new insight into magnetic energy scales and the resonance of the electron-doped side of the phase diagram [5].


3:06PM D2.00002 Quantum critical fluctuations in cuprates and d-wave superconductivity through their coupling to fermions, VIVEK AJI, University of California at Riverside — The phase diagram of the Cuprates is a collection of anomalies that has challenged our understanding of quantum many body physics. An organizing principle proposed to unify the experimental observations is the existence of a quantum critical point near optimal doping separating a phase which has broken time reversal and a renormalized Fermi liquid. I will discuss recent theoretical developments related to the nature of the fluctuations near the quantum critical point. The long wavelength theory of the time reversal violating state belongs to the dissipative 2DXY universality class. The fluctuation spectrum, at the quantum critical point, is local in space and power law in time, precisely of the form observed in the marginal fermi liquid phase near optimal doping. The fluctuations couple to the local angular momentum of the fermions to give a momentum dependence to the coupling which leads directly to pairing attraction in the d-wave channel. Theory of superconductivity in the cuprates, Vivek Aji, Arkady Shekhter and Chandra Varma, arXiv:0807.3741.

3:42PM D2.00003 Search for a thermodynamic evidence of a phase transition in the pseudogap state of YBa2Cu3O6+\( x \), BRIGITTE LERIDON, LPEM / CNRS — Recent polarized neutrons diffraction experiments have evidenced a symmetry breaking in the underdoped phase of superconducting cuprates [1,2,3]. This symmetry breaking takes place below a temperature \( T_{MAG} \) which increases when the number of charge carriers in the superconducting planes is decreased. We present here magnetic susceptibility measurements in YBa2Cu3O6+\( x \) ceramics. We have measured the magnetization of about twenty samples with different oxygen contents under 1T magnetic field. In some of them, we have observed an anomaly in the temperature derivative of the susceptibility at a temperature \( T_1 \) which seems to be in good agreement to the temperature \( T_{MAG} \). We show here the resulting phase diagram for underdoped YBa2Cu3O6+\( x \). These findings raise the question of a thermodynamic evidence for a phase transition in relation to the symmetry breaking observed by neutrons.


4:18PM D2.00004 Competition between the pseudogap and superconductivity in cuprates1, ADAM KAMINSKI, Ames Laboratory and Iowa State University — The relationship between the pseudogap and superconductivity is one of the central issues in physics of cuprates. By studying the spectral weights associated with pseudogap and superconductivity by angle resolved photoemission spectroscopy (ARPES) we found that there is a direct correlation between the loss of the low energy spectral weight due to the opening of the pseudogap and a decrease of the spectral weight associated with superconductivity as a function of momentum and doping. We therefore conclude that the pseudogap competes with the superconductivity by depleting the spectral weight available for pairing in the region of momentum space, where the superconducting gap is largest.

1This work was supported by Basic Energy Sciences, US DOE. The Ames Laboratory is operated for the US DOE by Iowa State University under Contract No. W-7405-ENG-82.
with different pairing strengths [2]. We observe that the gap magnitude variation is not determined by the electron-boson coupling but instead it is strongly
repulsion in these compounds? We quantitatively analyze the temperature evolution of the gap and the local electron-boson coupling for various atomic sites
with different pairing strengths [2]. We observe that the gap magnitude variation is not determined by the electron-boson coupling but instead it is strongly
correlated to variations present in the normal (ungapped) electronic states.


1This work was supported by NSF, DOE, PCCM-MRSEC.
time with coherent population trapping. The results are very encouraging: both the hole spin T1 and T2* times are surprisingly large.

A single electron in a nano-sized quantum dot is so strongly quantized that the interaction with the phonons is highly suppressed. This leads to potentially

This is accomplished via a canonical n-point function f_n, from which one can derive exact analytical expressions for any microstructural function of interest. This microstructural information can then be used to estimate accurately the bulk properties of the material. Unlike homogeneous materials, seemingly different bulk properties (e.g., transport and mechanical properties) of a heterogeneous material can be linked to one another because of the common microstructure that they share. Such cross-property relations can be used to estimate one property given a measurement of another. A recently identified decorrelation principle, roughly speaking, refers to the phenomenon that unconstrained correlations that exist in low-dimensional disordered materials vanish as the space dimension becomes large. Among other results, this implies that in sufficiently high dimensions the densest spheres packings may be ordered (rather than ordered) [S. Torquato and F. H. Stillinger, “New Conjectural Lower Bounds on the Optimal Density of Sphere Packings,” Experimental Mathematics, 15, 307 (2006)].

References

3:06PM D4.00002 Locking electron spins into resonance by electron-nuclear feedback\textsuperscript{1}, KATJA NOWACK, Delft University of Technology — All basic building blocks for spin-based quantum information processing using electron spins in GaAs quantum dots have recently been realized. Recent experiments have shown single-shot readout of an individual spin [1], the implementation of the SWAP gate [2] and (magnetically induced) coherent single electron spin rotations [3]. However, the main drawback of using electron spins in a GaAs environment is the short spin coherence time, which is measured to be in the nanosecond range [2,4]. The source of this fast decoherence is the hyperfine interaction of the localized electron spin with the randomly fluctuating nuclear spins of the host lattice. The fluctuations of the nuclear spins have to be reduced to extend the electron spin coherence time. We therefore study the electron-nuclear spin interaction and use magnetically driven spin resonance to control the electron spin and indirectly manipulate the nuclear spins. We apply continuous microwave excitation to the electron spin and observe strong electron-nuclear feedback. One experimental signature of this feedback is the locking of the electron spin system into resonance with the microwaves. Once the electron spin is locked into resonance, this coherence time. We therefore study the electron-nuclear spin interaction and use magnetically driven spin resonance to control the electron spin and indirectly manipulate the nuclear spins. We apply continuous microwave excitation to the electron spin and observe strong electron-nuclear feedback. One experimental signature of this feedback is the locking of the electron spin system into resonance with the microwaves. Once the electron spin is locked into resonance, this
4:54PM D4.00005 Dynamic nuclear polarization with single electron spins1. JACOB TAYLOR, Massachusetts Institute of Technology — Hyperfine interactions limit electron spin coherence times in GaAs quantum dots. By separating a spin singlet state on a chip, we measure an ensemble averaged spin dephasing time $T_2^*$ of 10 ns, limited by the contact hyperfine interaction with the GaAs host nuclei.$^2$ We use electrical control of the exchange interaction to drive coherent spin rotations. Exchange driven spin rotations are used to implement a “singlet-triplet spin echo” pulse sequence, which leads to a spin coherence time, $T_2$, exceeding 1 microsecond. We show that nuclear spins can be polarized by controlling two-electron spin states near the anti-crossing of the singlet ($S$) and triplet ($T_1$). An initialized $S$ state is cyclically brought into resonance with the $T_1$ state, where hyperfine fields drive rapid rotations between $S$ and $T_1$, “flipping” an electron spin and “flopping” a nuclear spin.$^3$ The resulting Overhauser field approaches 80 mT, in agreement with a simple rate-equation model. A self-limiting pulse sequence is developed that allows the steady-state nuclear polarization to be set using a gate voltage.

1In collaboration with J. Petta, M. Kolodrubetz, A. C. Johnson, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, A. C. Gossard. Financially supported by the Sloan Foundation, the David and Lucille Packard Foundation, and NSF DMR-0819860.


Monday, March 16, 2009 2:30PM - 4:54PM –
Session D5 FHP: Origins of Silicon Valley 401/402

2:30PM D5.00001 Prehistory of Silicon Valley, from 1910 to 1965. STEWART GILLMOR, Wesleyan University — The term "Silicon Valley" was coined in 1971, some six decades after the emergence of the San Francisco Bay Area as a center of innovation and invention in the fields of radio and electronics. The geographical position of San Francisco with respect to continental and Pacific transportation and communication needs; the growth of West Coast universities, markets, and population; the importation of talent from the East; innovative industrial and business methods—all these provided a thriving center of instrumentation, electronics, avionics, and high energy physics when Silicon arrived in the "Valley of the Heart’s Delight."

3:06PM D5.00002 W. W. Hansen, Microwave Physics, and Silicon Valley. DAVID LEESON, Stanford University — The Stanford physicist W. W. Hansen (b. 1909, AB ’29 and PhD ’32, MIT post-doc 1933-4, Prof. physics ’35-49, d. 1949) played a seminal role in the development of microwave electronics. His contributions underlay Silicon Valley’s postwar “microwave” phase, when numerous companies, acknowledging their unique scientific debt to Hansen, flourished around Stanford University. As had the prewar “radio” companies, they furthered the regional entrepreneurial culture and prepared the ground for the later semiconductor and computer developments we know as Silicon Valley. In the 1930’s, Hansen invented the cavity resonator. He applied this to his concept of the radio-frequency (RF) linear accelerator and, with the Varian brothers, to the invention of the klystron, which made microwave radar practical. As WWII loomed, Hansen was asked to lecture on microwaves to the physicists recruited to the MIT Radiation Laboratory. Hansen’s “Notes on Microwaves,” the Rad Lab “bible” on the subject, had a seminal impact on subsequent works, including the Rad Lab Series. Because of Hansen’s failing health, his postwar work, and MIT-Stanford rivalries, the Notes were never published, languishing as an underground classic. I have located remaining copies, and will publish the Notes with a biography honoring the centenary of Hansen’s birth. After the war, Hansen founded Stanford’s Microwave Laboratory to develop powerful klystrons and linear accelerators. He collaborated with Felix Bloch in the discovery of nuclear magnetic resonance. Hansen experienced first-hand Stanford’s evolution from its depression-era physics department to corporate, then government funding. Hansen’s brilliant career was cut short by his death in 1949, after his induction in the National Academy of Sciences. His ideas were carried on in Stanford’s two-mile long linear accelerator and the development of Silicon Valley.

3:42PM D5.00003 From Bell Labs to Silicon Valley: A Saga of Technology Transfer, 1954-1961. MICHAEL RIORDAN, UC Santa Cruz — Although Bell Telephone Laboratories invented the transistor and developed most of the associated semiconductor technology, the integrated circuit or microchip emerged elsewhere—at Texas Instruments and Fairchild Semiconductor Company. I recount how the silicon technology required to make microchips possible was first developed at Bell Labs in the mid-1950s. Much of it reached the San Francisco Bay Area when transistor pioneer William Shockley left Bell Labs in 1955 to establish the Shockley Semiconductor Laboratory in Mountain View, hiring a team of engineers and scientists to develop and manufacture transistors and related semiconductor devices. But eight of them—including Gordon Moore and Robert Noyce, eventually the co-founders of Intel—resigned en masse in September 1957 to start Fairchild, bringing with them the scientific and technological expertise they had acquired and further developed at Shockley’s firm. This event marked the birth of Silicon Valley, both technologically and culturally. By March 1961 the company was marketing its Micrologic integrated circuits, the first commercial silicon microchips, based on the planar processing technique developed at Fairchild by Jean Hoerni.

4:18PM D5.00004 The Origins and Development of the Silicon Valley Startup Model. JAMES GIBBONS, Stanford University — No abstract available.

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D6 DCOMP: Predictive Materials Design for Alternative Energy Storage 406

2:30PM D6.00001 First-Principles Studies of Phase Stability and Reaction Dynamics in Complex Metal Hydrides1. MEI-YIN CHOU, Georgia Institute of Technology — Complex metal hydrides are believed to be one of the promising materials for developing hydrogen storage systems that can operate under desirable conditions. At the same time, these are also a class of materials that exhibit intriguing properties. We have applied state-of-the-art computational techniques to study the structural, dynamic, and electronic properties of these materials. This talk will focus on the critical role played by the Ti catalyst in helping hydrogen cycling in the alanates, which remains a challenging topic for this hydrogen storage material. We have performed a series of calculations to address the hydrogen interaction on the aluminum surface in the presence of the Ti “dopant,” focusing on the effect of near-surface alloying on the Al(100) surface. It is found that Ti occupies subsurface sites near the Al surface. This subsurface Ti arrangement not only enhances H binding with the Al surface layer, but also improves H mobility on the surface. Based on existing experimental data and our preliminary results, we propose a model in which the catalyst does not enter the bulk, but facilitates hydrogen dissociation-recombination near the surface. In the dehydrogenation cycle, the catalyst kinetically facilitates the release and decomposition of AlH3 from the solid-state alanate. In the hydrogenation cycle, the catalyst helps the adsorption of hydrogen and the formation of AlH3 oligomers on Al surfaces. The implication of Ti as a catalyst for the hydrogenation reactions will be discussed.

1Supported by the Department of Energy.
3:06PM D6.00002 Energy Storage in Nanostructured Materials, YONG-HYUN KIM, National Renewable Energy Laboratory — Renewably produced energy by solar and wind technologies should be stored properly for practical use because of their intermittent generation of electricity. The energy can be stored in materials in forms of chemical, electrical, or thermal energies. The current energy-storage materials technologies, however, suffer from their inevitable low energy densities, compared to liquid fuels such as gasoline and ethanol, and thus end up to high cost due to material limitation. In order to overcome the fundamental limit, many scientists and researchers have studied nanostructured materials with more surface areas, tunable storage mechanisms, and better kinetic processes. Because electronic and mechanical properties of nanostructured materials are simply not a miniature of their bulk counterparts, a careful material design is required based on microscopic understanding of the energy storing process. In this talk, I will discuss our recent theoretical efforts and development to understand energy storage mechanisms in nanostructured materials for hydrogen, battery, and electrochemical capacitor applications. We have pioneered dihydrogen adsorption in nanostructured materials with the Kubas coordination [1-3] and lately developed efficient van der Waals potentials within the density functional theory approach [4]. Also very recently we have unraveled reversible lithium intercalation mechanisms in MoO3 nanoparticles for Li-ion battery electrodes [5], and been developing a microscopic theory of electrochemical and capacitive energy storage.


3:42PM D6.00003 Nanomaterials for Hydrogen Storage, PURU JENA, Virginia Commonwealth University — The success of a hydrogen economy critically rests on our ability to find materials that can store hydrogen with large gravimetric and volumetric densities and operate at near ambient conditions. To meet the large gravimetric density requirement, the storage materials must be lighter than Al. Unfortunately, in these light materials hydrogen is bound either too strongly or too weakly, thus leading to poor thermodynamics. I will discuss how the chemistry of these elements can be manipulated to bond hydrogen strongly and yet release it cleanly. The examples will include functionalized carbon fullerenes and nanotubes and doped AlN nanostructures. Using carbon nanostructures as catalysts I will demonstrate unambiguously the dehydrogenation mechanism of sodium alanate. A cluster perspective of the intermediate phases in the dehydrogenation of borohydrides will also be presented.

4:18PM D6.00004 Fundamental design of hydrogen storage structures and systems, ZHENHUI XIAO GUO, University College London — Fundamental simulations of hydrogen interactions with host structures offer indispensable insights to the understanding and design of hydrogen storage media for practical applications. First-principles approaches were applied to selected materials of high promise, e.g., doped/defective carbon, doped hydrides and metal/amine complexes. Several candidates show large capacities for hydrogen — over the 6.9 mass-percentage threshold considered for applications. Recent progress on carbon nanostructures show the importance of defects and doping on extra hydrogen uptake, and a small change of C-C interspacing on the mode-switching of hydrogen sorption. Work on the molecular analogues of the basic structural unit of boron-nitride indicates that transition metal (TM) atom doping can boost both the gravimetric and thermodynamic capacities of hydrogen in these materials. The H2 binding to the TM dopants is Kubas-like in nature, though the maximum binding capacity at the TM doped sites does not follow the 18-electron rule. Progress in the Li-N-H system shows that the N-Li bond is weaker than the N-H bonds in LiNH2, and consequently LiNH2 can dissociate into Li+ and (NH2)-, or (LiNH)- and H+. Hence, of NH3 may evolve as a transient gas, if it is not sufficiently captured by a reactive component, e.g. LiH. Molecular dynamics calculations indicate that hydrogen delivery is possible close to fuel-cell operation conditions. Comparison is also made with experiment where possible.

4:54PM D6.00005 First principles design of electric-field-assisted high capacity hydrogen storage media, MINA YOON, Oak Ridge National Laboratory, Fritz-Haber-Institut der Max-Planck-Gesellschaft, University of Tennessee — Hydrogen has been viewed as a highly appealing energy carrier for renewable energy. To achieve economic feasibility hydrogen storage materials with high gravimetric and volumetric densities must be developed. However, no materials so far satisfy the essential criteria for economically feasible hydrogen storage. Therefore, there are necessities of breakthrough ideas and methods for developing new materials. In this talk, I will discuss the novel idea of electric-field-assisted hydrogen storage in nanostructures. Its central ingredient is to create high and strongly delocalized electric fields that are strong enough to attract hydrogen through polarization. Using quantum mechanical first-principles calculations, it has been shown that high electric fields can be easily established in a region close to the surface of nanostructures by electronic doping [1] or in charge compensated ways. The charging idea and its underlying physical mechanism can be generalized to many other related nanoscale materials that are of interest for hydrogen storage, as exemplified by alkaline-earth-metal coated carbon nanostructures [2] and charge transferred organic crystals [3].


Monday, March 16, 2009 2:30PM - 5:30PM — Session D7 GSNP: Rare Events in Physics and Population Dynamics 407

2:30PM D7.00001 Transitions in the Kramers escape rate in classical and quantum field theories, DANIEL STEIN, New York University — Small random fluctuations, either of thermal or quantum origin, are the cause of many important and interesting physical phenomena. These include chemical reactions, nucleation in phase transitions (i.e., the formation of a droplet of one phase within another phase), and the formation of unusual spatially localized states in various condensed matter systems. In all of these, random fluctuations (or “noise”), no matter how small, eventually drives a physical system from one stable state to another. We discuss how in some classical systems thermally activated hopping over a barrier undergoes a transition as an external parameter such as system size or external field is varied. Its features are similar to those arising when classical activation over a barrier crosses over to quantum tunneling through that barrier as temperature is lowered. This crossover has some (but not all of the) features of a second-order phase transition. We also discuss two timely applications from mesoscopic physics: thermally induced breakup of monovalent metallic nanowires, and stochastic reversal of magnetization in thin ferromagnetic annuli. Each are of interest both from the point of view of fundamental physics and for potential technological applications.

1. Research partially supported by NSF PHY-0651077.
Further work is needed to theoretically account for the observed behavior. Also in this configuration, moreover, the frequency and lineshape of these oscillations exhibit periodicity as a function of externally applied magnetic flux. Variety of dynamical effects, including self-sustained oscillations, stochastic resonance, and intermittency between different steady-state and limit-cycle solutions. Duffing-like nonlinearity of the mechanical beams is well understood, the piecewise-linear behavior exhibited by the superconducting stripline resonators is yet using two classes of systems, namely, nanomechanical resonators in the form of doubly clamped beams, and electromagnetic resonators made of superconducting striplines. While a bifurcation between monostable and bistable zones is employed for the first class of resonators, a bifurcation between monostable and astable perturbations. This behavior can be exploited for amplifying small signals, and also for noise reduction (squeezing). We experimentally demonstrate these effects.

Accurate predictions. Moreover, the time of occurrence (i.e., phase) of an outbreak proves to be a useful new parameter that carries important epidemiological contrasts with the well known Rossler oscillator whose outbreaks recur regularly but whose amplitude vary chaotically in time (Uniform Phase Chaotic Amplitude the chaotic regime. In fact, it is difficult if not impossible to locate realistic chaotic parameter regimes in which outbreaks occur regularly each year. This and predict years in which the epidemic is absent rather than outbreak years. Skipping events are intrinsic to the forced SIR model when parameterised in the model’s natural oscillations. The analysis advanced here attempts to make progress in this direction by focusing on the dynamics of “skips” where we identify and predict years in which the epidemic is absent rather than outbreak years. Skipping events are intrinsic to the forced SIR model when parameterised in the chaotic regime. In fact, it is difficult if not impossible to locate realistic chaotic parameter regimes in which outbreaks occur regularly each year. This contrasts with the well known Rossler oscillator whose outbreaks recur regularly but whose amplitude vary chaotically in time (Uniform Phase Chaotic Amplitude oscillations). The goal of the present study is to develop a “language of skips” that makes it possible to predict under what conditions the next outbreak is likely to occur, and how many “skips” might be expected after any given outbreak. We identify a new threshold effect and give clear analytical conditions that allow accurate predictions. Moreover, the time of occurrence (i.e., phase) of an outbreak proves to be a useful new parameter that carries important epidemiological information. In forced systems, seasonal changes can prevent late-initiating outbreaks (i.e., having high phase) from running to completion. These principles yield forecasting tools that should have relevance for the study of newly emerging and reemerging diseases.

Research in part supported through NSF-DMR 2008.

Recent papers:


The author acknowledges support from ONR and ARO.
2:30PM D8.00001 Thermal Spin Transfer Torques1, GERRIT BAUER, TU Delft — The coupling between spin and charge in electronic transport is studied in the field of spintronics. Heat currents are coupled to both charge and spin currents as well [1]. This extension of spintronics to what may be called “spin caloritronics” recently enjoys renewed attention [2]. The spin-transfer torque associated with electric currents can excite magnetizations in nanostructures, switching magnetic configuration in spin valves and move domain walls in magnetic wires when exceeding critical values of the order of $10^4$ A cm$^{-2}$ [3]. Also heat currents transfer spin angular momentum [4], either intrinsically or via the thermo-electric generation of particle spin currents. We predict that temperature differences of the order of 100 K over typical metallic nanostructures cause effects equivalent to the critical charge current densities. In this talk I will give a brief review of various aspects of spin caloritronics with emphasis on thermal spin transfer torques. This work has been carried out in collaboration with Moosa Hatami, Qinfang Zhang, Paul Kelly, Hans Joakim Skadsem, Arne Brataas and Sadamichi Maekawa.

1Supported by NanoNed and the EC project DynaMax.

3:06PM D8.00002 Nonequilibrium intrinsic spin torque in a single nanomagnet1, AURELIEN MANCHON, University of Arizona — The spin transfer torque usually observed in metallic and tunneling spin-valves, as well as magnetic domain walls, comes from the transfer of the transverse spin-current of conduction electrons to the magnetization [1]. Therefore, it requires both a non collinear configuration of the magnetic structure (or inhomogeneous magnetic texture in the case of domain walls) and magneto-resistive effects. However, a number of magnetic systems show magneto-resistive effects in a single magnetic layer, such as anisotropic magnetoresistance (AMR) [2]. In the presence of spin-orbit interaction (SOI) the electron scattering depends on the magnetization direction. Recent theoretical studies suggest that in such systems, a transverse component of the spin density builds up, due to the spin-dependent scattering introduced by the spin-orbit coupling. Consequently, a transverse spin density arises from intrinsic properties of the band structure without the need of non-collinear magnetization. In the case of a single ferromagnet with spin-orbit interaction, the exchange interaction between the accumulated spin and the magnetization gives rise a spin torque on the magnetization. We show that this torque can be used to control the magnetization direction injecting current densities as low as $10^5$-10$^6$ A/cm$^2$, comparable or lower than the spin transfer effect. We first study the general case of a single ferromagnetic layer with spin-orbit interaction and then focus on the cases of effective Hamiltonians, such as Rashba and Dresselhaus SOI, as well as Luttinger hole systems. We discuss the relation between the spin torque and the spatial inversion symmetry of various forms of spin-orbit couplings and compare this spin torque with the conventional spin transfer torque. We finally discuss several magnetic systems for possible experimental realizations. This work was done in collaboration with Shufeng Zhang. [1] J.C. Slonczewski, J. Magn. Magn. Mater. 159, L1 (1996); L. Berger, Phys. Rev. B 54, 9353 (1996). [2] T.R. McGuire and R.I. Potter, IEEE Trans. Mag. 11, 1018 (1975).

3:42PM D8.00003 Spin transfer torques in antiferromagnets and magnetic semiconductors, PAUL HANEY, National Institute for Standards and Technology — Spin transfer torques (STT) in ferromagnetic metals can be understood in terms of conservation of total spin, allowing a simple evaluation and interpretation of these torques in terms of spin currents. STTs also occur in antiferromagnets, which have no net spin and different symmetries than ferromagnets, resulting in qualitatively different torques. We consider a structure with a compensated antiferromagnetic layer and a ferromagnetic layer. We find a STT on both layers, which vanishes when the layers' order parameters are either collinear or perpendicular. This torque can drive the magnetization of a thin film ferromagnet to be perpendicular to the easy plane. In dilute magnetic semiconductors, strong spin orbit coupling in the semiconductor host implies that spin is not even approximately conserved, requiring modifications of the microscopic calculation of the STT. We describe these modifications and present results from first principles calculations of STT in GaMnAs.

4:18PM D8.00004 Spin-Transfer-Torques at a Ferromagnet/Antiferromagnet Interface1, MAXIM TSOI, Physics Department, University of Texas at Austin — Spintronics in ferromagnetic systems is built on a complementary set of phenomena in which the magnetic configuration of the system influences its transport properties and vice versa. Giant magnetoresistance (GMR) [1] and spin- transfer-torque (STT) [2] phenomena are typical examples of such interconnections. Recently, MacDonald and co-workers [3] predicted that corresponding effects ought to occur in systems where ferromagnetic (F) components are replaced by antiferromagnets (AFM). I will present our experimental search for these new AFM effects which may potentially lead to a new all-antiferromagnetic spintronics where antiferromagnets are used in place of ferromagnets. In particular I will focus on our experiments with exchange-biased spin valves [4] where extreme current densities were found to affect the exchange bias at F/AFM interface [5-7]. As exchange bias is known to be associated with interfacial AFM magnetic moments, our observation can be taken as the first evidence of STT effect in AFM materials.


4:54PM D8.00005 Effects of polarizer dynamics on current-induced behaviors in magnetic multilayer nanopillars1, SERGEI URAZHDIN, West Virginia University — Magnetic nanodevices usually include two magnetic layers - a polarizing “fixed” layer, and a “free” layer, whose roles are determined by their relative thicknesses. I will describe our measurements of spin transfer in nanopillars with similar thicknesses of the “polarizer” and the “free” layer. In the first sample type, both layers were patterned into similar lateral dimensions. Spectroscopic measurements of current-induced dynamics showed incoherent bipolar excitations. Thermally-activated reversal statistics exhibited dependences on magnetic field and applied current dramatically different from the “standard” samples with a thick polarizing layer. I will also discuss our results for samples in which only the free layer was patterned into a nanopillar, while the polarizing layer was left extended with dimensions of several micrometers. These samples exhibit coherent precession of only the extended layer, only the polarizer, or both, depending on the relative thicknesses of the two layers. The transition between the “free”-like and “fixed”-like behaviors of each layer occurred over a small range of thickness. I will show that current-induced behaviors of our samples can be understood in terms of the dynamical coupling between ferromagnets induced by spin transfer. This coupling can result suppression of the current-induced precession, incoherent dynamics, or for certain geometries in enhancement of current-induced dynamics in magnetic bilayers.

1Supported by NSF DMR-0747609 and a Cottrell Scholar Award from the Research Corporation.
2:30PM D9.00001 Can one hear a Kolmogorov Spectrum?1, SERGIO RICA, LPS, CNRS-Ecole Normale Supérieure — I will talk about a work in collaboration with G. Durrin and C. Josserand on the long-time evolution of waves of a thin elastic plate in the limit of small deformation so that modes of oscillations interact weakly. According to the theory of weak turbulence (successfully applied in the past to plasma, optics, and hydrodynamic waves), this nonlinear wave system evolves at long times with a slow transfer of energy from one mode to another. We derived a kinetic equation for the spectral transfer in terms of the second order moment. We show that such a theory describes the approach to an equilibrium wave spectrum and represents also an energy cascade, often called the Kolmogorov-Zakharov spectrum. We perform numerical simulations that confirm this scenario. Finally, I will discuss recent experiments by A. Boudaoud and collaborators and N. Mordant.

1Agence Nationale de la Recherche (ANR)

2:42PM D9.00002 Dynamical Origami, CHRISTOPHE JOSSE, ARNAUD ANTKOWIAK, BASILE AUDOLY, SÉBASTIEN NEUKIRCH, Institut D’Alembert, CNRS & UPMC, INSTITUT D’ALEMBERT TEAM — A drop falling on a thin elastic sheet is rapidly trapped after impact by self-folding of the sheet around the drop. This trapping process, due to capillary forces, occurs on the fast timescale of hydrophobic rebound. The resulting packed drop presents a complex three-dimensional shape, characteristic of the interplay between elasticity and capillarity (Py et al., Phys. Rev. Lett. 98, 2007). We study experimentally the encapsulation dynamics with high-speed video camera. A shape selection exhibited by the system is evidenced. The role played by the different parameters of impact (drop radius, impact velocity...) in the final shape of this “dynamical origami” is eventually discussed.

2:54PM D9.00003 Mass distribution and geometry of a crumpled ball, ANNE DOMINIQUE CAMBOU, NARAYANAN MENON, UMass, Amherst — We use X-ray CT scanning to resolve in 3-dimensions the conformation of aluminum sheets with diameters L=7cm to 10cm and thickness T=25 microns, crumpled into spheres with diameters D=1.2cm to 1.5cm. The linear resolution of the reconstructed images is less than 6 microns/voxel. Measurements were made on spheres with average volume fractions, φ ranging from 0.06 to 0.11. The mass is not homogeneously distributed in the volume: when averaged over several samples, the volume fraction d(L/D) is found to increase with radius so that the sphere is densest at its surface. The radial dependence of volume fraction appears to be independent of average volume fraction and diameter, D. We also report preliminary measurements of the distribution of curvature in the sphere.

3:06PM D9.00004 Stress relaxation in thin crumpled sheets, INGO DIERKING, PAUL ARCHER, University of Manchester — Compression of thin crumpled sheets subjected to a constant weight shows a wide range of scaling, covering up to five orders of magnitude [1], i.e. time scales from seconds to weeks. We demonstrate that this scaling behaviour is not smooth, but rather interrupted by sudden changes in height of the uniformly compressed crumple, which we attribute to sudden ridge collapses. Interestingly, when plotting the time laps between successive discontinuous ridge collapses as a function of time, the data falls onto a single linear functionality for all polymer film thicknesses, with a slope of dΔt/dt=1 over a scaling regime of four orders of magnitude.[2] Further, we investigate the scaling behaviour of thin sheets of different metals to elucidate a possible relation between the scaling parameter and the Young’s modulus. Preliminary experiments suggest that scaling is a linear function of the elastic modulus. [1] K. Matan, R.B. Williams, T.A. Witten, S.R. Nagel, Phys. Rev. Lett., 88, (2002), 076101. [2] I. Dierking, P. Archer, Phys. Rev. E, 77, (2008), 051608.

3:18PM D9.00005 The compensation of Gaussian curvature in developable cones is local, JIN WANG, THOMAS WITTEN, The James Franck Institute and The Department of Physics, The University of Chicago — We use the angular deficit scheme[1] to determine numerically the distribution of Gaussian curvature in developable cones(d-cones)[2] formed by forcing a flat elastic sheet into a circular container so that the sheet buckles. This provides a new way to confirm the vanishing of mean-curvature[3] at the rim where the sheet touches the container. This angular deficit scheme also allows us to explore the potential role of the Gaussian-Bonnet theorem in explaining the mean-curvature vanishing phenomenon. The theorem's global constraint on curvature resembles the global conditions observed to be relevant for vanishing mean curvature. However, our result suggests that the Gauss-Bonnet theorem does not explain the vanishing of mean-curvature.


3:30PM D9.00006 Buckling Thin Disks and Ribbons with Non-Euclidean Metrics, CHRISTIAN SANTANGELO, UMass Amherst — I consider the problem of a thin membrane on which a metric has been prescribed, for example by lithographically controlling the local swelling properties of a polymer thin film. While any amount of swelling can be accommodated locally, geometry prohibits the existence of a global strain-free configuration. To study this geometrical frustration, I introduce a perturbative approach. I compute the optimal shape of an annular, thin ribbon as a function of its width. The topological constraint of closing the ribbon determines a relationship between the mean curvature and number of wrinkles that prevents a complete relaxation of the compression strain induced by swelling and buckles the ribbon out of the plane. These results are then applied to thin, buckled disks, where the expansion works surprisingly well. I identify a critical radius above which the disk in-plane strain cannot be relaxed completely.

3:42PM D9.00007 Fragmentation of an elastica, NICOLAS VANDENBERGHE, EMMANUEL VILLERMAUX, IRPHE, CNRS - Aix Marseille Universite — When a thin rod is submitted to an axial force greater than its critical buckling load it takes the shape of an elastica. As the load further increases, a rod made of a brittle material breaks suddenly. More than two fragments may be formed during this fragmentation. In this work we discuss the sequence of events that lead to the final broken state with two or more fragments. We show that the criterion for breaking is not trivial. In particular, we investigate the effect of the duration of the loading and we show that at a given load the waiting time before breaking is broadly distributed. We discuss the consequences of the time delayed breaking on the distributions of fragment sizes and fragment numbers.
3:54PM D9.00008 Relaxation of a plastic fold1, MORGAN CERVO, NARAYANAN MENON, U. of Massachusetts, Amherst — Crumpled objects have been observed to show stress relaxation when confined to a constant volume, and to show creep when subjected to a constant load. These relaxation processes are described by logarithmic (or other similarly slow) functional dependences on waiting time. In an effort to understand the microscopic elements responsible for this slow collective relaxation, we study the mechanics of a single fold in a thin strip of polycarbonate sheet (typical dimensions: thickness t=0.127 mm, length L=14 cm, and width w=2cm). We create folds of different initial opening angles by placing the strip under varying loads. We then measure the opening angle as a function of time. We find that even one isolated fold is sufficient to mimic the relaxation behavior of the composite crumpled sheet: the unfolding process is logarithmic in time. The unfolding rate depends on sheet thickness, but surprisingly is independent of initial opening angle. We have observed qualitatively similar behavior in metal and paper sheets.

1Supported by NSF DMR 0606216 and NSF MRSEC DMR-0820506

4:06PM D9.00009 Shape and trajectory of a tumbling elastic sheet of paper1, MIKE ROBITAILLE, ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA 01610 — Inspired by wind dispersal of winged seeds and gliders, we study the flight of a tumbling piece of paper to explore the competing effect of inertia, lift, drag, and elasticity on its aerodynamics. Above a critical aspect ratio, a rigid rectangular sheet is well known to exhibit autorotation, leading to a lift force which causes it to drift away from the vertical as it falls through air. Less known is that the fact that the sheet buckles and bends along the axis of rotation when the rigidity of the sheet is reduced. We measure the deflection of the paper as a function of aspect ratio, and find its speed and angle of descent with high speed imaging. We find that the rotation speed is lower when the sheet is bent, than when it is unbent. The sheet deflection increases above a critical aspect ratio reaching a maximum before decreasing. The angle of descent is well described by a simple model balancing the gravitational, lift and drag forces acting on the sheet.

1In collaboration with Daniel Tam and John Bush (MIT).

4:18PM D9.00010 Shape and trajectory of a tumbling elastic sheet of paper II, DANIEL TAM, MIT, MICHAEL ROBITAILLE, ARSHAD KUDROLLI, Clark University, JOHN BUSH, MIT, DEPARTMENT OF MATHEMATICS, MIT TEAM, DEPARTMENT OF PHYSICS, CLARK UNIVERSITY TEAM — We investigate the dynamical coupling between the tumbling motion and elastic deformation of a paper strip freely falling in air. Recent experiments suggest the existence of a critical length above which the strip bends as it tumbles. We demonstrate that this bending is caused by the centripetal force associated with its tumbling motion. A simple theory predicts that bending occurs above a critical length in much the same way that buckling occurs in a compressed beam. We further discuss the influence of bending on the trajectory of paper strips, as well as biological implications for the dispersal of seed pods.

4:30PM D9.00011 Nonlinear response of tensed membranes, PEEKER MILAS, BENNY DAVIDOVITCH, Physics Dept., UMass Amherst — We study the response of elastic membranes under tension T, to localized normal forces F. Focusing on simple geometries, characterized by translational or radial symmetries, we calculate the membrane shape for a range of values of F and T by numerically solving the appropriate FvK equations. We find that the linear regime, where membrane displacement is proportional to F, vanishes in the asymptotic limit FT ≪ 1, and characterize scaling properties of the resulting nonlinear response. We discuss the relevance of our results to the puzzling scaling behavior of the length of radial wrinkles, recently found in “drop on membrane” experiments (Huang et al. Science 2007).

4:42PM D9.00012 Period Fissioning and Other instabilities of stressed elastic membranes, BENNY DAVIDOVITCH, Physics Dept., UMass Amherst — We study the shapes of elastic membranes under the simultaneous exertion of tensile and compressive forces when the translational symmetry along the tension direction is broken. We predict a multitude of novel morphological phases in various regimes of a 2-dimensional parameter space (ε, ν), defined by the relevant mechanical and geometrical conditions. The parameters ε, ν are, respectively, the ratio between compression and tension, and the wavelength contrast along the tension direction. In particular, our theory associates the repetitive period fissioining pattern, recently observed on wrinkled membranes floating on liquid and subject to capillary forces (J. Huang et al.) to the morphology in the asymptotic regime (ε ≪ 1, ν ≫ 1) where tension is dominant and the wavelength contrast is large.

4:54PM D9.00013 Experimental study of the dynamics of crumpling, HILLEL AHARONI, ERAN SHARON, Hebrew University in Jerusalem — We experimentally measure the temporal evolution of crumpled configurations of thin elastic sheets. In our experiment, elastic hydrogel sheets swell inside a hard spherical shell, free of gravitational and plastic effects. We observe the dynamic evolution of structures in the sheet as confinement ratio increases, and analyze the statistical nature of the elastic energy localization along singularities.

5:06PM D9.00014 Geometry Induced Charge Separation on a Helicoidal Ribbon, AVADH SAXENA, Los Alamos National Lab, VICTOR ATANASOV, Bulgarian Academy of Sciences, ROSSEN DANDOLOFF, Universite de Cergy-Pontoise, GEOMETRY AND NONLINEARITY COLLABORATION — Helical ribbons are ubiquitous in nature including in the carbon based nanostructures such as graphene. We derive an effective geometry-induced quantum potential for a particle confined on a helicoidal ribbon. This potential leads to the appearance of localized states at the rim of the helicoid. In this geometry the twist of the ribbon plays the role of an effective transverse electric field on the surface and thus this is reminiscent of the quantum Hall effect. We also calculate the effective polarization and discuss the consequences of these findings.

Monday, March 16, 2009 2:30PM - 5:30PM – Session D10 DMP: Focus Session: Ferroelectrics III and Piezoelectrics 304

2:30PM D10.00001 Light scattering answers precisely to the soft-mode in PbTiO3 paraelectric phase, HWEE PING SOON, HIROKI TANIGUCHI, YASUHIRO FUJII, MITSURU ITOH, Tokyo Institute of Technology (Materials and Structures Laboratory), MAKOTO TACHIBANA, National Institute for Materials Science — PbTiO3 (PT) acts solely as the long-standing textbook example for the displacive-type phase transition; however, the precise observation of the soft-mode behavior of PT paraelectric phase still remains unavailable although it has been addressed by many research works [1-4]. In this study, we revisit the soft-mode behavior of PT single crystal by the confocal micro-Raman measurements. Opposing to the conventional belief that there occurs no first-order Raman scattering in the centrosymmetric PT paraelectric phase, the temperature dependence of the soft-mode has been precisely resolved for the first time due to the existence of macroscopic size Raman active regions (≥ 780 nm). By evidently ruling out the possibility of defect-induced Raman scattering, the elasto-optical coupling serves as the most likely mechanism for the occurrence of these Raman active regions. [This work was supported by both Kakenhi (Grant No. 20248098) and Global COE program.] [1] G. Shirane, J. D. Axe, and J. Harada, Phys. Rev. B 2, 155 (1970). [2] M. Kempa et al., Phase Trans. 79, 351 (2006). [3] N. E. Tornberg and C. H. Perry, J. Chem. Phys. 53, 2946 (1970). [4] M. D. Fontana, H. Idrissi, and K. Wojcik, Europhys. Lett. 11, 419 (1990).
2:42PM D10.00002 Pretransitional Diffuse Neutron Scattering in Ferroelectric KTa$_{1-x}$Nb$_x$O$_3$

GRACE YONG, Towson University, ROSS ERWIN, NIST Center for Neutron Research, OLEKSII SVITELSKYI, University of Alberta, JEAN TOULOUSE, Lehigh University, LYNN BOATNER, Oak Ridge National Laboratory, BERNARD HENNION, Laboratory Leon Brillouin, STEPHEN SHAPIRO, Brookhaven National Laboratory — Pretransitional diffuse neutron scattering in ferroelectric KTa$_{1-x}$Nb$_x$O$_3$ occurs at (110), (111), and (130) with no diffuse scattering at (100), and (200). These observations will be discussed using the elastic structure factor and ‘uniform phase shift’ description.

2:54PM D10.00003 Nonlinear Driven Response of a Phase-Field Crystal in a Periodic Pinning Potential

CRISTIAN ACHIM, TTK, Finland, JORGE RAMOS, INPE, Brazil, MIKKO KARTTUNEN, University of Western Ontario, Canada, KEN ELDEN, Oakland University, ENZO GRANATO, INPE, Brazil, TAPIO ALA-NISSILA, TTK, Finland, SEE-CHEN YING, Brown University — We study numerically the phase diagram and the response under a driving force of the phase field crystal model for pinned lattice systems in one and two dimensions. The model describes the lattice system as a continuous density field in the presence of a periodic pinning potential, allowing for both elastic and plastic deformations of the lattice. We first present results for phase diagrams of the model in the absence of a driving force. The nonlinear response to a driving force on an initially pinned commensurate phase is then studied via overdamped dynamic equations of motion for different values of mismatch and pinning strengths. For large pinning strength the driven depinning transitions are continuous, and the sliding velocity varies with the force from the threshold with power-law exponents in agreement with analytical predictions. Transverse depinning transitions in the moving state are also found in two dimensions. Surprisingly, for sufficiently weak pinning potential we find a discontinuous depinning transition with hysteresis even in one dimension under overdamped dynamics. We also characterize structural changes of the system in some detail close to the depinning transition.

3:06PM D10.00004 Mesoscopic nanostructures and long-time relaxation processes in ferroelectrics with coexisting ferroelectric and antiferroelectric phases

V. SOBOLEV, South Dakota School of Mines & Technology, Rapid City, South Dakota 57701, USA, V. ISCHUCH, Institute for Single Crystals of the Academy of Sciences of Ukraine, Kharkov 61001, Ukraine, Z. SAMOILENKO, Physics/Engineering Institute of the Academy of Sciences of Ukraine, Donetsk 83114, Ukraine — Presentation contains results of experimental study of the kinetics of mesoscopic segregated structures formed in the vicinity of interphase domain boundaries separating the domains of the coexisting ferroelectric and antiferroelectric phases in two series of the lead zirconate titanate based solid solutions in which the isovalent complex (La$_{3+}$,$\La^{3+}$)$_2^{2+}$ or the La$^{3+}$ ions are substituted for lead. These systems of solid solutions possess an extended interval of compositions for which the inhomogeneous state of coexisting ferroelectric and antiferroelectric domains is energetically favorable in comparison with homogeneous ferroelectric and antiferroelectric phases. The mechanisms that control the kinetics of formation of the segregates are investigated and compared for these two series of solid solutions.

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3:18PM D10.00005 Accurate calculations of the full NMR chemical shielding tensor in perovskites: B3LYP embedded cluster results for $^{17}$O and $^{47,49}$Ti

DANIEL L. PECHKIS$^2$, ERIC J. WALTER, HENRY KRAKAUER, College of William and Mary — B3LYP calculations of $^{17}$O and $^{47,49}$Ti NMR in BaTiO$_3$ and SrTiO$_3$ will be presented. These systems were modeled with finite size quantum clusters embedded in classical fields generated from arrays of point charges and pseudopotentials. For polar clusters, an external E-field was applied to eliminate spurious depolarization fields. The full $^{17}$O chemical shielding tensors, $\sigma(O)$, in BaTiO$_3$ and SrTiO$_3$ are in very good agreement with recent precise single crystal measurements. The calculated Ti isotropic chemical shielding values are within the range of all reported measurements of BaTiO$_3$. Results will also be presented for the solid solution PZT series.

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3:30PM D10.00006 Local ordering and structural instabilities in (Na,Bi)TiO$_3$ perovskites

SAHAK PETROSYAN, Massachusetts Institute of Technology, MARCO FORNARI, Central Michigan University, BORIS KOZINSKY, Bosch GmbH, NICOLA MARZARI, GERBRAND CEDER, Massachusetts Institute of Technology — Density functional theory is used to predict structural and electronic properties of lead-free piezoelectric perovskite (Na,Bi)TiO$_3$. Prediction of the energetics of different phases in the phase diagram and investigated the tendency to local ordering on the A-site. In order to elucidate the mechanism for the phase transitions and the piezoelectric performance we also probed the dependence of ferrodistortive and antiferrodistortive instabilities upon pressure and chemical substitutions. Our results point to local tetragonal ordering and provide insight on possible structural changes of the system in some detail close to the depinning transition.

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3:42PM D10.00007 Density-functional study of the Ba$_{1+2x}$Bi$_{(1-x)}$(M$_{1-x}$)$_2$Ti$_{(1+x)/2}$O$_3$ perovskite solid solution

DENNIS JACKSON, Oregon State University, DAVID ROUNDY, Oregon State University — Using density-functional theory we predict properties of the solid solution perovskites Ba$_{1+2x}$Bi$_{(1-x)}$(M$_{1-x}$)$_2$Ti$_{(1+x)/2}$O$_3$ where M is Mg, Ni or Zn. These properties are strongly affected by the presence of both A-site and B-site disorder. We study all distinct orderings within a given supercell. Results will also be presented for the solid solution PZT series.

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3:54PM D10.00008 Predicting new structures in B-cation ordering perovskites

MATTHEW LORDS, Brigham Young University — Material properties are intimately tied to crystal structure. Many materials, alloys in particular, share a common, underlying motif, such as an fcc, bcc, or hcp parent lattice but have different chemical orderings on the lattice. For example, the well-known structure in the Cu-Au system, L1$_0$, has an underlying fcc lattice where each (001) plane contain only Cu or Au. The planes are stacked so that the Cu and Au layers alternate. Among the countably infinite possibilities for such chemical orderings, why does nature choose only the few it does? Are others possible or likely? We answer this question generally and give an example of the perovskite structure, important in ferroelectrics, catalysts, and superconductors. We show which structures are possible combinatorially and which might actually be observed in real materials.

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4:06PM D10.00009 First principles study of piezorotation in thin-film LaAlO$_3$

ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — We investigate the effect of biaxial strain on [001] thin-film LaAlO$_3$ using density functional calculations. We find that the essentially rigid rotations of the AlO$_6$ octahedra vary linearly with strain, a phenomenon which may be described as piezorotation by analogy with piezomagnetism or piezoelectricity [S. Denev, et al., Phys. Rev. Lett. 100, 257601 (2008)]. Within a small range of experimentally achievable strain values, we find that epitaxial strain can stabilize several distinct modes of cooperative rotations not found in the bulk, and identify first order phase transitions between states with different piezorotative responses. Finally, we investigate how the electronic and elastic properties are affected by proximity to the strain-induced phase transitions.
4:18 PM D10.00010 - Nano-electromechanical systems based on a piezoelectric single crystalline thin film on Silicon. JONGHOO PARK, DUSTIN J. KREFT, ROBERT H. BLICK, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706, SEUNG-HYUB BAEK, CHANG-BEOM EOM, Department of Material Science and Engineering, University of Wisconsin-Madison, WI 53706, V. VAITHYANATHAN, Department of Material Science and Engineering, Pennsylvania State University, PA 16802, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Cornell University, NY 14853, VLADIMIR AKSYUK, Alcatel-Lucent Technologies, NJ 07974 — Nano-electromechanical systems (NEMS) have shown great progress and promise as sensors and actuators. In spite of great progress, efficiency and integration techniques for actuating and tuning NEMS have remained a challenge. We have employed a single crystalline piezoelectric thin film on a silicon substrate to obtain a high piezoelectric coefficient and high electromechanical coupling for a NEMS device. The suspended NEMS device consists of Pt/Pb(Mg0.33Nb0.67)O3/PbTiO3/SrRuO3/SiO2 and is clamped at the ends via silicon substrate. Pt and SrRuO3 are used as top and bottom electrodes, respectively, and SiO2 serves as a buffer layer to the silicon substrate. We have shown experimentally that the piezoelectric actuation based on PMN-PT devices consume less power and are more responsive than other NEMS devices of similar nature and size.

4:30 PM D10.00011 - Structural Study of PMN-xPT by Neutron Diffraction. D. PHELAN, P.M. GEHRING, Q. HUANG, NIST, Z.-G. YE, Simon Fraser, C. STOCK, ISIS, G. XU, J. WEN, Brookhaven — Stark differences between x-ray and neutron measurements of the structures of ferroelectric-relaxors PMN-xPT (1-x)Pb(Mg1/3Nb2/3)O3+xPbTiO3 and PZN-xPT (Z=Zn) have been reported [1]. One explanation for these differences is that these crystals have strained surface layers on the order of several tens of µm thick, the crystal structure of which differs from that of the crystal bulk. This phenomenon may have been coined the “anomalous skin effect” but has been recently challenged [2] and thus remains controversial. We re-investigated the skin effect in PMN-xPT by considering the possibility that the oxygen stoichiometry might play a role. Two sets of powders (x=0.1, 0.2, 0.3, and 0.4) were grown, one with and one without oxygen annealing, and high resolution neutron powder diffraction measurements were carried out for both sets. For a given x, both sets of powders have the same structural phase, suggesting that the effects of oxygen annealing are minimal. For x=0.1 and x=0.2 both sets of powders are rhombohedral, which contrasts with the single crystal neutron neutron diffraction measurements. This supports a skin effect in that the grain size of the powders is small enough that the Bragg peaks are dominated by the strained surface layer. References [1] G. Xu et al., Phase Transitions 79, 135 (2006) [2] E. H. Kisi and J.S. Forrester, J. Phys.:Condens. Matter 17, L381 (2005)

4:42 PM D10.00012 - Complex local structures in lead based pervoskite relaxors. GUANGYONG XU, ZHU XIU, JINSHE WEN, Brookhaven National Lab, PETER GEHRING, NIST, CHRIS STOCK, RAL, U.K. — The lead-based, pervoskite relaxors Pb(Zn1/3Nb2/3)O3 (PZN), Pb(Mg1/3Nb2/3)O3 (PMN) and their solid solutions with PbTiO3 (PT) continue to receive significant attention because they exhibit huge piezoelectric responses and are therefore technologically important. It is widely accepted that many of the special properties of relaxors are related to local (charge, chemical, and polar) order. In particular, short-range polar order, a.k.a. “polar nano-regions” (PNR), is believed to appear in relaxors at temperatures well above the Curie temperature Tc. The PNR contribute to the frequency dispersion of the dielectric properties and have recently been suggested to be associated with the high piezoelectric response. We have performed series of neutron diffuse scattering measurements on PMN-xPT and PZN-xPT single crystals. Our results indicate that the local polar structure is complicated, having T1 and T2-type components with different polarizations. In particular, the T1 component with [001] polarization can be partially suppressed by an [001] field, the T2 component with [110] polarization can be affected by a [111] field. The T2 component also exhibits a strong coupling to the acoustic phonon while the T1 component is associated with the polar optic phonon. We will discuss the complex nature of the local structure in relaxors and their implications.

4:54 PM D10.00013 - First-Principles Study of Diffuse Scattering in Pb(SC1/2Nd1/2)O3. P. GANESH, M. AHART, R.E. COHEN, Geophysical Laboratory, Carnegie Institute of Washington, E. COCKAYNE, B. BURTON, Materials Science and Engineering Laboratory, NIST — Recent X-ray and neutron experiments show diffuse scattering with characteristic butterfly and rod shapes in relaxor ferroelectrics Pb(SC1/2Nd1/2)O3 (PSN) and Pb(Zn1/3Nb2/3)O3 (PZN) [1]. We have simulated diffuse scattering in PSN using first-principles based simulations in the ferroelectric, relaxor and the paraelectric phases [2]. The model assumes quenched chemical order in the form of chemically ordered regions in a chemically disordered matrix. Below the Burns temperature, polar nanoregions (PNR) form, pinned spatially to the COR, but whose polarization evolve dynamically. In the relaxor phase we find “butterfly” shaped diffuse scattering around the [100] peaks and around the [110] peaks we find “rod” shaped diffuse scattering similar to experiments. As the system is driven towards the paraelectric phase, the diffuse patterns around all the Bragg peaks display radial streaks elongated towards the origin. We have determined that the rods and butterflies below the Burns temperature originate from the PNR, while the radial streaks above it arise from atomic displacements associated with chemical disorder. References: [1] G. Xu, Z. Zhong, H. Hiroka and G. Shirane, Phys. Rev. B, 70, 174109 (2004) [2] S. Tinte, B. P. Burton, E. Cockayne and U. V. Waghmare, Phys. Rev. Lett. 97, 137601 (2006)

5:06 PM D10.00014 - High-pressure x-ray diffraction and Raman scattering studies of Pb(Mg1/3Nb2/3)O3-xPbTiO3. MUKHTAR AHART, MADDURY SOMAYAZULU, RONALD COHEN, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington — Motivated to determine and understand the compositional-pressure phase diagram for PMN-xPT solid solutions, we employed the angular dispersive x-ray diffraction methods (Advanced Photon Source, Argonne National Laboratory) and high pressure Raman scattering to investigate a series of PMN-xPT solid solutions (x=0.2, 0.3, 0.33, 0.37, 0.4) in a diamond anvil cell up to 20 GPa. The x-ray diffraction results show changes in Bragg peaks at about 6 or 7 GPa which indicate that PMN-xPT systems undergo a ferroelectric to a paraelectric phase transition. In addition, a new peak centered at 380 cm-1 appears above 6 GPa for all the samples. The morphotropic phase boundary (x=0.33 to 0.37) with the monoclinic symmetry persists up to 7 GPa. Based on our results, we propose a possible structure for high pressure phase, which is R3c. We suggest a phase diagram for PMN-xPT system which is slightly different from the one predicted by B. Chaubane et al (Phys. Rev. B 70, 134114, 2004).

5:18 PM D10.00015 - Molecular dynamics computational studies of relaxor ferroelectric behavior in Pb(Mg1/4Ti1/4Nb1/2)O3 (PMN-PT). HIROYUKI TAKENAKA, ILYA GRINBERG, ANDREW RAPPE — Relaxor ferroelectrics are of fundamental scientific interest and are also used in a variety of applications, such as piezoelectric transducers and capacitors. They exhibit permittivity peaks that are broad with respect to both temperature and frequency. We have developed a bond-valence model for Pb(Mg1/4Ti1/4Nb1/2)O3 (PMN-PT) and performed atomistic bond-valence molecular dynamics (BVMD) simulations of PMN-PT. We have studied relaxor behavior at a range of temperatures, in order to analyze polar nanoregion dynamics and relaxation lifetimes. We find that even for a fairly small simulation size of 6×6×6 supercell (1080 atoms), the system exhibits frequency dispersion. We present the results of 6×6×6, 8×8×8 and 10×10×10 supercell BVMD simulations, analyze the pair distribution function of the PMN-PT and elucidate the local chemical origin of relaxor behavior.
2:30PM D11.00001 Robust Ferromagnetism in type-II (ZnMn)Te Quantum Dots . I.R. SELLERS1, V.R. WHITESIDE, M. EGINLIGIL, R. OSZWALDOWSKI, I. ZUTIC, A. PETROU, B.D. MCCOMBE, University at Buffalo, W.C. CHOU, National Chiao Tung University, Taiwan — Temperature dependant magneto-photoluminescence studies of type-II diluted magnetic semiconductor (ZnMn)Te/ZnSe quantum dots (QDs) will be presented. As expected, the exchange interaction between the Mn spins and charge carriers results in a strong optical polarization of the luminescence at low temperature in a magnetic field. In addition, however, a zero magnetic field optical polarization degree of 7% is observed in the photoluminescence (PL). This polarization is shown to be independent of temperature until 180 K, and is only quenched by the loss of PL intensity as the type-II QDs are ionized. In this submission, we will present continuous wave and temporal PL measurements which indicate that the finite polarization, at zero magnetic field results from the formation of excition magno polarons (EMPs). Furthermore, we will show that these EMPs are remarkably robust with binding energies in excess of 40 meV, far larger than typical of the widely studied EMP system. The origin of this behavior will be discussed. Work supported in part by CSEQuIn and the Office of the Provost at the U. Buffalo.

1current address: Sharp Research Laboratories Europe, Oxford, UK

2:42PM D11.00002 Low threshold amplified spontaneous emission and Auger recombination suppression in giant nanocrystal quantum dots . ISTVAN ROBEL, FLORENCIO GARCIA-SANTAMARIA, RICHARD D. SCHALLER, YONGFEN CHEN, JENNIFER A. HOLLINGSWORTH, VICTOR I. KLIMOV, Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Nanocrystal quantum dots (QDs) are attractive materials for various light-emitting applications including optical amplification and lasing. A complication associated with the multiexciton nature of light amplification is NQDs is the picosecond optical-gain decay induced by nonradiative Auger recombination, in which one exciton recombinates by transferring the energy to the other. Here, we present new results on a novel type of nanocrystals dubbed “giant” quantum dots (g-QNDS). These g-QNDS comprise an emitting core particle of CdSe overcoated with a thick shell (up to 20 monolayers) of wider-gap CdS. We report that biection and gain lifetimes are greatly augmented and the ASE threshold drops down to just a few μJ/cm2. We explain this result by a significant increase in the absorption cross-section of g-QNDS compared to traditional nanocrystals and lengthening of biection lifetimes. We also observe other unusual optical-gain behaviors for these structures such as multi-band ASE, the spectra spectral range of optical amplification extends over more than 500 meV. These results demonstrate that g-QNDS are very promising materials for applications in practical lasing technologies.

2:54PM D11.00003 Investigation of group-III-nitride semiconductor nanostructures using an eight-band k · p formalism . OLIVER MARQUARDT, TILMANN HICKEL, JOERG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung — Despite its approximative nature, the k · p formalism provides a numerically efficient and accurate description of the electronic structure of group-III nitride semiconductor nanostructures with characteristic size of a few nanometers. [1] With the computational effort of this method being independent of the system size, it is possible to study an extensive set of zero-, one- and two-dimensional nanostructures. We applied a plane-wave implementation of the 8-band k · p formalism and second-order continuum elasticity theory to various III-nitride nanostructures such as InGaN/GaN or GaN/AlN quantum dots in the characteristic wurtzite and zincblende crystal structures. We investigated the effect of strain and polarization effects on the charge carrier localization which typically leads to a spatial separation of electrons and holes in wurtzite nanostructures. Additionally, studies have been performed in order to evaluate trends when varying the alloy composition in InGaN/GaN nanostructures in order to understand light emission processes in realistic nanostructures.


3:06PM D11.00004 Infrared Photodetectors based on PbSe and PbS Nanoparticles . DON-HYUNG HA, University of Pennsylvania, Department of Materials Science and Engineering, CHRISTOPHER MURRAY, University of Pennsylvania, Department of Chemistry and Materials Science and Engineering — There is growing interest in developing nanoparticles for photodetectors, due to the potential to selectively tune the wavelengths detected by varying the size of the nanoparticles. Also, by virtue of the solution processibility of nanoparticles, photodetectors based on nanoparticles provide a low cost, easily processed opportunity for photodetection on flexible substrates. Especially for the near-infrared (NIR) region, PbS and PbSe nanoparticles are ideal candidates since their absorption windows fall between 900-1500nm and 1400-2500nm, respectively, covering a wide range of the IR region. This presentation reports the synthesis, structural characterization, and photoconductivity of colloidal PbSe and PbS nanoparticles. Photocurrent and normalized detectivity are measured from the nanoparticle photodiode under the illumination of NIR light (800-2500 nm) and under dark conditions.

3:18PM D11.00005 Single photon to single electron conversion using a quantum dot . HARUKI KIYAMA, TAKAFUMI FUJITA, Department of Applied Physics & QPEC, the University of Tokyo, TETSUYA ASAYAMA, Advanced Materials Laboratories, Sony Corporation, AKIRA OIWA, SEIGO TARUCHA, Department of Applied Physics & QPEC, the University of Tokyo — Photons, and electron spins are leading candidates for implementing quibits useful in information transmission, and computing, respectively. Therefore, quantum media conversion (QMD) between them is a key technology for a comprehensive quantum network. In this work, as a first step toward QMD, we demonstrate single photon to single electron (charge) conversion using a GaAs based lateral QD equipped with a quantum point contact (QPC) as a charge sensor. A distinctive step, which is quite similar to those observed for single electron tunneling onto the QD from the leads, is observed in the single-shot time evolution of the QPC current immediately after the incidence of single photons. From detailed measurements of the light intensity dependence and the QD-lead tunnel rate dependence we confirm that the observed steps are due to single photon generation in the QD just after single photon irradiation. The minimum time resolution of this single photon to single electron conversion is 50 μs. This is short enough to demonstrate the angular momentum transfer between photon polarization and electron spin in the QD as the next step.

3:30PM D11.00006 Scalable Single Photon Detector for Terahertz and Infrared Applications . BERNARD MATIS, DONG HO WU, Naval Research Laboratory — Recent advancements in the research areas of quantum dot (QD) and single electron transistors (SET) open up an exciting opportunity for the development of nanostructure devices. Of the various devices, our attention is drawn in particular to detectors, which can respond to a single photon over a broad frequency spectrum, namely, microwave to infrared (IR) frequencies. Here we report on transport measurements of parallel quantum dots, fabricated on a GaAs/AlGaAs 2-dimensional electron gas (2DEG) substrate, under the influence of external fields associated with 110GHz and 1 THz signals. We further investigate the scalability of our detector in addition to its temperature dependence up to 4.2K. We will discuss experimental results, and their dependence on quantum dot size, and fabrication techniques, as well as the limitations in developing a QD photon detector for microwave and IR frequencies, whose noise equivalent power can be as high as 10⁻²² W/Hz¹/².

3:42PM D11.00007 Measurement of the separation dependence of the resonant energy transfer between CdSe nanocrystallite quantum dots . FARBOD SHAFIEI, RICARDO S. DECCA, Indiana University-Purdue University Indianapolis — An apparatus has been built to study the separation dependence of the interaction between small and large resonant groups of CdSe/ZnS nanocrystallite quantum dots (NQDs). A near-field scanning optical microscope (NSOM) is used to bring a group of mono-disperse 6 nm dots close (near-field range) to an 8 nm group of dots which are deposited on a solid immersion lens. Combination of spectral and positional filtering allows us to measure the interaction between small numbers of NQDs, with the ultimate goal of identifying the interaction between individual dots. Quenching of the small NQDs photoluminescence signal yields the transition probability between these two groups of NQDs which is obtained to be (4.5×10⁻²⁷ m⁶/γ/R⁵), matching the theoretical calculation. Förster radius as a signature of energy transfer efficiency is extracted from experimental data to be 17 nm. Separation between two groups of the NQDs was increasing up to 40nm during the experiment.
Resonant excitation in coupled InAs/GaAs quantum dots.

3:54PM D11.00008 Resonant creation of a positive trion in coupled InAs/GaAs quantum dots.

SWATI RAMANATHAN, KUSHAL C. WIJESUNDARA, MAURICIO GARRIDO, ERIC A. STINAFF, Department of Physics and Astronomy, Ohio University, A. S. BRACKER, D. GAMMON, Naval Research Laboratory — Recent photoluminescence excitation (PLE) experiments have revealed the unexpected resonant creation of a positive trion in a coupled InAs/GaAs quantum dot system. Positive trion creation is a two photon process requiring the second photon to have a different energy from the first due to the presence of the photogenerated hole. This leads us to conclude that the positive trion may be created through two indirect absorptions, along with two tunneling events. To verify this scenario, experiments using circularly polarized excitation should result in hole spin states with either spin -3/2 or +3/2. This should lead to Pauli blocking of spins, resulting in a reduced intensity of positive trion emission under excitation with circularly polarized light when compared to unpolarized light. High resolution PLE will also provide additional insight into the details of this mechanism. It may be possible to use resonant excitation processes such as this to create defined hole spin states in coupled quantum dot systems.

4:06PM D11.00009 Exchange interactions in coupled quantum dots observed through polarized photoluminescence.

KUSHAL C. WIJESUNDARA, MAURICIO GARRIDO, SWATI RAMANATHAN, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701, USA, ALLAN BRACKER, D. GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — Identification and manipulation of the exchange interaction between different spin configurations may be useful for implementing quantum logic operations. Coupled quantum dots offer the possibility of controlling the exchange interaction by continuously tuning between direct and indirect excitonic configurations. The effect of the anisotropic part of the exchange energy was clearly identified from polarization dependent photoluminescence (PL) results arising from the direct and indirect configurations of the neutral exciton. We also observe direct experimental evidence of the isotropic exchange interaction via PL measurements from positive trion configurations. The isotropic exchange interactions observed to be an order of magnitude larger than the anisotropic splitting as expected. High resolution measurements of these charged exciton configurations are expected to reveal additional insight into the details of the exchange interaction.

4:18PM D11.00010 Hybrid Exciton in a Semiconductor Nanorod Coated By an Organic Shell.

DANIEL VELAZQUEZ, HUONG NGUYEN, Marshall University — We study the Wannier Mott-Frenkel hybrid exciton in a nanorod coated by a thin organic shell. Using the wavefunctions of the 1D Wannier-Mott and the Frenkel exciton, we obtain the wavefunctions and energy of the hybridization state. The new exciton state is a linear combination of the basic exciton states and is smoothly distributed over the whole system. The hybridization depends strongly on the coupling (hybridization) parameter as well as the shape of the nanorod and the thickness of the organic layer.

We also observed that there exists a threshold pump laser power which separates the linear and super-linear regions. The effective pump power can be as low as demonstrated to increase as the lengths of nanowire segments decreases. As far as the relationship between Raman scattering intensity and laser pump power, we believe our observation suggests the possibility to make a new type of SRS semiconductor laser.

This work is supported by NSF NIRT, grant DMR-0304178.

4:30PM D11.00011 Stimulated Raman Scattering from Short GaP Nanowires.

JIAN WU, AWNISH GUPTA, PETER EKLU ND, DEPARTMENT OF PHYSICS TEAM, DEPARTMENT OF MATTERIAL SCIENCE AND ENGINEERING TEAM — We report an interesting discovery of very strong non-linear optical behavior in short GaP nanowire segments. They were formed by cutting a ~40 µm long and 210 nm diameter GaP nanowire into various lengths using a focused ion beam. This approach allows us to study length as the variable in the non-linear behavior. A giant nonlinear Raman amplification has been observed in these segments with length L < 1.2µm for the first time. The nonlinear Raman effect has been demonstrated to increase as the lengths of nanowire segments decreases. As far as the relation between Raman scattering intensity and laser pump power, we also observed that there exists a threshold pump laser power which separates the linear and super-linear regions. The effective pump power can be as low as 200 µW that is 1000 times smaller than bulk values. We attribute this giant nonlinear Raman effect to stimulated Raman scattering (SRS) from nanocavities formed by these short GaP nanowires. The quality factor Q of these short segments was estimated to be 10^3 to 10^4. We believe our observation suggests the possibility to make a new type of SRS semiconductor laser.

4:42PM D11.00012 Polarized Rayleigh and Raman Study of single CuO Nanowire.

QIUJIE LU, JIAN WU, HUMBERTO GUTIERREZ, TIMOTHY RUS S, Department of Physics, The Pennsylvania State University, PETER EKLU ND, Department of Physics and Department of Material Sciences, The Pennsylvania State University — Crystalline CuO is an interesting Ferroelectric and Ferromagnetic system which we have recently grown in nanowire (NW) form. In this paper, we present results of Raman and Rayleigh scattering studies of individual CuO NWs to probe optical antenna effects that we first discovered in GaP NWs. We have shown that these antenna effects can, in general, strongly mask Raman selection rules in semiconducting nanowires[1]. Using a microRaman spectrometer, polarized light scattering experiments (backscattering geometry) were carried on NWs suspended over holes in a TEM grid. TEM images were used to identify the NW diameters. As a function of the angle θ between the NW axis and the incident laser field, we collect the Rayleigh scattering intensity as well as the Raman LO and TO optical phonon scattering intensity. These results can then be used to quantify the optical antenna effects in the CuO system. NWs of different diameters, from 70nm to 200 nm were studied; the results depend dramatically on the NW diameter. Our results will be compared to EM calculations based on the DDA approximation. This work is supported by NSF NIRT, grant DMR-0304178. [1] Chen G. Jian Wu, etc., Nano Lett. 2008 Vol.8 pp. 1341-1346.

4:54PM D11.00013 Polarized Rayleigh and Raman Back-scattering from Individual GaP Nanowires.

DUMING ZHANG, JIAN WU, QIUJIE LU, HUMBERTO GUTIERREZ, PETER EKLU ND, Department of Physics, The Pennsylvania State University — Results of polarized Rayleigh and Raman back-scattering studies are reported for individual ~20 µm long crystalline GaP Nanowires (NWs) using 514.5 nm excitation. The NWs were supported over holes in TEM grids. The diameters and growth directions of the NWs were thereby determined by TEM and the samples were studied optically. Peak positions of LO, TO phonon bands were found to agree with bulk GaP. Both the Rayleigh and Raman back-scattering intensity polar patterns I(θ) were measured at room temperature, where θ is the angle between the incident electric field and the NW axis. The scattered radiation was polarized parallel to the incident electric field. From the Rayleigh back-scattering intensity polar patterns, the factor in the scattered radiation was obtained. Together with the Raman tensor determined from the growth direction of the NWs, the Raman back-scattering intensity polar pattern was calculated for each case and correlated with the experimental data. Our measurement on the Rayleigh and Raman back-scattering intensity polar patterns revealed different patterns ranging from dipole-like to symmetric (circular or elliptical) depending on the NWs growth directions and diameters. This work is supported by NSF NIRT, grant DMR-0304178.


WO SEOK CHOI, SOON JAE MOON, Seoul National University, HIROMICHI OHTA, Nagoya University, BYUNG CHEOL JEON, JONG HOON SHIN, Seoul National University, YUN SANG LEE, Soongsil University, TAE WON NOH, Seoul National University — Recently, oxide heterostructures are being extensively investigated as an effort to understand unusual physics occurring at the oxide interfaces. For example, formation of 2DEG or strongly modified electronic structures at the interface between two different oxide constituents have been examined carefully and understood to some extent. In this contribution, we studied the electronic properties and phonon dynamics of Nb:SnTiO$_3$/SrTiO$_3$ superlattices. Using optical spectroscopy, we obtained the optical conductivity for a wide range of photon energy (3.7 meV – 6 ev). We could separately identify the free carrier response and the phonon dynamics of the superlattice. The carrier density and unusually small scattering rate were obtained varying temperature as well as the superlattice period. In addition, we could reveal a strong electron-phonon coupling from the existence of the spectral weight in mid-IR photon range.

This work is supported by NSF NIRT, grant DMR-0304178.
5:18PM D11.00015 Effect of Magnetic Field on Broadening of Excitonic Spectra in Superlattices1. YURI KHAVIN, NIKOLAI SIBELDIN, MIKHAIL SKORIKOV, VITALY TVSETKOV, P.N. Lebedev Physical Institute, RAS, Moscow, Russia, DANIEL OBERLI, ALOK RUDRA, ROMAIN CARRON, ELI KAPON, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland — We present a comprehensive study of optical properties of GaAs/AlGaAs superlattices (SLs) with different tunneling coupling between wells in magnetic fields in a wide range of excitation levels. Photoluminescence (PL) and PL excitation spectra demonstrate significant broadening of the exciton lines with increasing excitation power. Several features indicate that the exciton line widths are mainly determined by excitonic scattering. In particular, in zero magnetic field, the heavy hole (hh) PL line broadens symmetrically with increasing excitation power. In nonzero in-plane magnetic field, the exciton binding energy strongly increases (by a factor of 2 in 14 T), and the dependence of the line width on excitation power becomes much weaker. In strong in-plane fields, significant shift of the hh PL line towards lower energies is observed under high excitation levels. It is possible that this shift is a manifestation of interparticle interactions in an electron-hole system.

1Supported by the RFFR (project no. 08-02-01438) and by the project SCOPES 2005-2008.

Monday, March 16, 2009 2:30PM - 5:30PM — Session D12 DMP DCMP: Novel Instrumentation and Techniques in Surface Science 308

2:30PM D12.00001 A Combined Scanning Tunneling Microscope-Quartz Crystal Microbalance Investigation of Heating and Liquid-Like Behavior at a Sliding Interface1. BENJAMIN DAWSON, JACQUELINE KRIM, North Carolina State University — The unique capabilities resulting from combining a scanning tunneling microscope and a quartz crystal microbalance have been used to characterize the heating and wear at the interface of a tungsten tip and an Indium substrate, with a change in the contact characteristics of the interface occurring for sufficient sliding speeds. The advantage of this system is the ability to probe subtle changes of a rubbing asperity contact, which will aid in developing a more complete understanding of the complex issue of heat generated via friction.

1This work funded by the AFOSR Extreme Friction MURI Grant FA9550-04-1-0381.

2:42PM D12.00002 Dynamics and Spreading of pentanol and other alcohols for MEMS applications1. BRENDAH MILLER, DAVID HOOK, JACQUELINE KRIM, North Carolina State University — Microelectromechanical Systems (MEMS) have the potential to revolutionize widespread technologies, but tribological issues are currently preventing commercialization of some devices. Self-assembled monolayers (SAMs), while highly effective against release related stiction, are ineffective as MEMS lubricants [1]. Vapor phase lubrication has been proposed as a solution to the issue of tribological failure in MEMS with alcohol vapors attracting much interest. In an effort to understand the basic mechanisms of lubrication we have performed a quartz crystal microbalance (QCM) study of the uptake, sliding friction, and spreading rates of adsorbed alcohols on silicon and SAM treated substrates. [1] D. A. Hook, S. J. Timpe, M. T. Dugger, and J. Krim. Tribological degradation of fluorocarbon coated silicon microdevice surfaces in normal and sliding contact. J. Applied Physics 104 (2008).

1Funded by AFOSR Extreme Friction MURI Grant #FA9550-04-1-0381.

2:54PM D12.00003 Numerical Studies of Friction Between Metallic Surfaces and of its Dependence on Electric Currents1. EVANGELOS MEINTANIS, MICHAEL MARDER, Center for Nonlinear Dynamics, The University of Texas at Austin — We will present molecular dynamics simulations that explore the frictional mechanisms between clean metallic surfaces. We employ the HOLA molecular dynamics code to run slider-on-block experiments. Both objects are allowed to evolve freely. We recover realistic coefficients of friction and verify the importance of cold-welding and plastic deformations in dry sliding friction. We also find that plastic deformations can significantly affect both objects, despite a difference in hardness. Metallic contacts have significant technological applications in the transmission of electric currents. To explore the effects of the latter to sliding, we had to integrate an electrodynamics solver into the molecular dynamics code. The disparate time scales involved posed a challenge, but we have developed an efficient scheme for such an integration. A limited electrodynamics solver has been implemented and we are currently exploring the effects of current in the friction and wear of metallic contacts.

1Funded by the Institute for Advanced Technology at The University of Texas at Austin.

3:06PM D12.00004 Combined conducting atomic force/scanning Kelvin probe microscope for investigating charge trapping on semiconductor surfaces. JAMES MOORE, SEAN KENNY, Longwood University, MONIKA RUCHALA, MIKHAIL RESCHCHIKOV, ALISON BASKI, Virginia Commonwealth University — A novel combination of conducting atomic force microscopy (CAFM) and scanning Kelvin probe microscopy (SKPM) was used to investigate charge trapping and transfer on semiconductor surfaces. CAFM is first used to locally inject charge at an oxide/semiconductor interface, and then SKPM is performed to monitor the evolution of the resulting surface potential. In a dark environment, the additionally charged interface states due to CAFM charge injection result in additional band bending that persists for hours in GaN, ZnO and Si. Specifically for GaN, a model based on a tunneling mechanism was used to describe the CAFM charge injection, where electrons travel from the tip through an oxide barrier and become trapped at the interface. The decrease in induced band bending with time shows a logarithmic behavior, similar to transients produced after exposure to light. This combination of techniques offers a relatively simple method for investigating induced band bending on semiconductor surfaces and could become a useful tool for understanding concentrations of charged surface states. Specifically, current collapse in GaN FETs and HFETs has been linked to concentrations of charged surface states at the contacts.

3:18PM D12.00005 Hot Electron Transport Properties of Thin Copper Films Using Ballistic Electron Emission Microscopy, J.J. GARRAMONE, J.R. ABEL, I.L. SITNITSKY, University at Albany, L. ZHAO, I. APPELBAUM, University of Delaware, V.P. LABELLA, University at Albany — Copper is widely used material for electrical interconnects within integrated circuits and recently as a base layer for hot electron spin injection and readout into silicon. Integral to both their applications is the knowledge of the electron scattering length. To the best of our knowledge, little work exists that directly measures the scattering length of electrons in copper. In this study we used ballistic electron emission microscopy (BEEM) to measure the hot electron attenuation length of copper thin films deposited on Si(001). BEEM is a three terminal scanning tunneling microscopy (STM) based technique that can measure transport and Schottky heights of metal/semiconductor systems. We find a Schottky height of 0.67 eV and an attenuation length approaching 40 nm above the Schottky height at 77 K. We also measure a decrease in the attenuation length with increasing tip bias to determine the relative roles of inelastic and elastic scattering.
3:30PM D12.00006 A Comparative Study of Au-Au, Ru-Ru and RuO\textsubscript{2}-Au RF MEMS Contacts in Controlled Vacuum Environments\textsuperscript{1}, MATTHEW WALKER, J. KRIM, N. MCGRUER, North Carolina State University — We have constructed an UHV system with in situ oxygen plasma cleaning capabilities in order to observe the impact of film contamination in reproducible conditions. We have performed measurements to allow comparison of soft, hard and combined soft-hard contacts. All switches are closed before applying a potential across the contacts to minimize e-field evaporation and material transfer between contacts. Prior to, and for short O2 plasma exposure times, the initial contact resistance measurements had larger variations. With longer O2 plasma exposure times initial and extrapolation resistances measurements converged. These results are consistent with prior reports, which showed that the oxide layer on a Ru surface thickens with exposure to O2 plasma \cite{1}. Therefore, under stringent experimental conditions, we have demonstrated that operating RF MEMS contacts are comparable to those studied in the surface science literature. \cite{1} Y. Iwasaki, A. Izumi, H. Tsurumaki, A. Namki, H. Oizumi, I. Nishiyama, Appl. Surf. Sci. 253, 2007

3:42PM D12.00007 Reduction of Barrier Height at Close Proximity between two Gold (111) surfaces.\textsuperscript{1}, YOSHIHIKO KURIYAMA, TOKYO Institute of Technology — Work function is one of important physical properties in order to understand electron emission or chemical reactions such as catalysis. Work function changes locally depending on a defect, step or adsorbate on the surface. A scanning tunneling microscope (STM) is one of powerful tools to investigate such a local work function, which is called a local barrier height. In this method, the barrier height is defined as $\phi = (1/1.025 \times \ln(G/dz)^2$, where G is conductance and z, the tip-surface distance. Experimentally, the barrier height has been reported to be constant independent of the distance. But, theoretically, it is suggested to be reduced at close proximity. In this study, we investigated the distance between two gold (111) surfaces in TEM observation simultaneously with measuring conductance value in a process of approaching each other. The distance changes controllably by a piezo actuator when it is above 1 nm, but the distance becomes narrower that the expected value obtained by a piezo actuator when it is below 1 nm. Obviously, structural relaxation is occurred when the distance between two gold surfaces is below 1 nm. Taking the structural relaxation into an account, we confirm that the barrier height is reduced at close proximity of two gold (111) surfaces. \textsuperscript{1}PRESTO-JST

3:54PM D12.00008 Coherent X-ray Surface Diffraction: Speckle from the Surface Reconstruction Layer of Gold (001), MICHAEL S. PIERCE, KEE-CHUL CHANG, DANIEL HENNESSY, Argonne National Laboratory, Materials Science Division, ALEC SANDY, MICHAEL SPRUNG\textsuperscript{1}, Argonne National Laboratory, Advanced Photon Source, HOYDOO YOU, Argonne National Laboratory, Materials Science Division — We present preliminary results of the first coherent x-ray diffraction from an atomic monolayer surface reconstruction and demonstrate how this technique is capable of providing new information about surface dynamics. Speckled scattered patterns were successfully collected from ordered surface atoms on Au (001) crystals in high vacuum. We have collected data at the (001) anti-Bragg point as well as coherent scattering data directly from the in-plane hex reconstruction peak. These two points can provide complementary information about in-plane and out-of-plane surface dynamics. Below 1050 K, the system appears to remain in equilibrium maintaining a small constant fraction of non-reconstructed surface for a given temperature. However we observe the speckles continue to evolve within the collected scattering patterns indicating that the non-reconstructed portion of the surface rearranges slowly. Above about 1050K, we find that the rate of speckle decorrelation rapidly increases for very small changes in temperature. Signal to noise makes this a difficult experiment with existing light sources. However we expect this technique to become easier and more broadly applicable with future X-ray sources.

4:06PM D12.00009 In-situ chemical and structural characterization via RHEED-total reflection analysis of x-rays (TRAXS).\textsuperscript{1}, SANDEEP CHANDRIL, CAMERON KEENAN, THOMAS MYERS, DAVID LEDERMAN, West Virginia University — The use of x-ray fluorescence produced inside a molecular beam epitaxy chamber by the RHEED electron gun to simultaneously characterize the thin films for thickness, roughness and the chemical composition is described. This technique requires only slight modifications to the chamber and can be a powerful tool for beam flux calibration and in-situ analysis, especially where surfaces have to be protected under vacuum and for the stoichiometry control during growth. The angular dependence of the x-ray fluorescence signal from the thin film over the substrate is analyzed using Parratt’s approach and simulating electrons’ trajectories inside the film to account for grazing angle electron beam as a source for x-rays. We have found good agreement between the experiment and the theory for the thickness and roughness estimates. Experiments for chemical composition determination are currently underway. \textsuperscript{1}This work was funded by the Office of Naval Research (Grant N00014-02-1-0974), the Air Force Office of Scientific Research (MURI grant FA9550-03-0-0330), and the National Science Foundation (CIAM-DMR grant 0502825).

4:18PM D12.00010 High Energy XRD/XRF for High-Throughput Phase Mapping of Composition Spread Thin Films\textsuperscript{1}, JOHN GREGOIRE, DARRENT DALE, ALEXANDER KAZIMIROV, MICHELE TAGE, HECTOR ABRUNA, FRANCIS DISALVO, R. BRUCE VAN DOVER, Cornell University — Analysis of thin film inorganic libraries is an increasingly popular technique for materials discovery. Due to the high throughput nature of thin film epitaxy, the high throughput nature of the x-ray beam and the high spatial resolution of x-ray fluorescence, x-ray techniques provide a powerful tool to determine the composition of thin films. As the landscape of thin film material discovery grows, the ability of x-ray techniques to provide high spatial resolution mapping for a large number of samples becomes increasingly important. We present recent progress towards high energy x-ray characterization of thin film phase purity and composition spread films. This work is supported by the Cornell Fuel Cell Institute (DOE award DE-FG02-03ER46072) and the Cornell High Energy Synchrotron Source (NSF award DMR-025180).

4:30PM D12.00011 Low Energy Electron Microscope Imaging of Doped Si Structures Buried under Thermal Oxides\textsuperscript{1}, GARY KELLOGG, MEREDITH ANDERSON, CRAIG NAKAKURA, Sandia National Laboratories — We present recent progress towards low energy electron microscope (LEEM) imaging of doped-silicon, diode test structures buried under thermally grown oxides. The question addressed here is whether the observed contrast at incident electron energies just above the vacuum cutoff is due to differences in doping type or oxide thicknesses. To circumvent complications arising from charging of the when exposed to the imaging electron beam, we developed a method to measure “pre-charging” current voltage (IV) curves and applied it to three test samples with oxide thicknesses varying from 2.8 to 50 nm. The vacuum cutoff energies obtained from the IV curves depend on both doping type and oxide thickness and are strongly influenced by external factors including surface contamination and UV exposure. The time dependence of the oxide charging increases significantly with oxide thickness providing further insights into the origins of LEEM contrast.

\textsuperscript{1}Sandia is operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. DOE’s NNSA under Contract No. DE-AC04-94AL85000.
4:42PM D12.00012 LEED structural analysis of strongly correlated systems: reaching the limit of the instrumentation?  
Teyu Chienn, Biao Hu, Dept. of Physics & Astronomy, U. of TN, Knoxville, Shuheng Pan, Dept. of Physics, U. of Houston, V. Braun Nascimento, E. Ward Plummer, Dept. of Physics & Astronomy, LSU — In strongly correlated systems, like transition-metal oxides and the Iron Pnictides, subtle changes in structural parameters can cause dramatic changes in the physical properties. Breaking the symmetry by creating a surface is a controlled way to explore the structure-functionality relationship. Low Energy Electron Diffraction (LEED) I – V has been one of the most used surface structural techniques, but there are inherent and instrumental limitations which will be discussed using data from surfaces of transition-metal compounds. Using CCD cameras and new data analysis three dimensional plots of diffraction vs parallel momentum can be created. Spot intensity, width, position, and profile, as well as the diffuse background can then be quantitatively extracted and evaluated. We will show how to couple the STM with LEED using data from the parent superconducting compound BaFe2As2. The inherent limitations of the existing system are tested using Cu(100).

4:54PM D12.00013 Electron emission from surfaces resulting from low energy positron bombardment1, S. Mukherjee, K. Shastry, A. H. Weiss, U. Texas at Arlington — Measurements of the energy distribution of electrons resulting from very low energy positron bombardment of a polycrystalline Au and Cu(100) surfaces provide evidence for a single step transition from an unbound scattering state to an image potential bound state. The primary positron energy threshold for secondary electron emission and cutoff in the secondary electron energy spectra are consistent with a process in which an incident positrons make a transition from a scattering state to a surface-image potential bound while transferring all of the energy difference to an outgoing secondary electron. Estimates of the probability of this process as a function of incident positron energy are also presented. Background free Auger spectra of the MVV transition in Cu and the OVV transition in Au were obtained by setting the incident positron beam energy below the secondary electron emission threshold. Auger electron emission resulted from the annihilation of surface state positrons with core electrons. The low energy tail associated with the low energy CVV Auger transitions in Cu and Au were found to have integrated intensity several times larger than Auger peak providing strong evidence for multi-electron Auger processes.

5:06PM D12.00014 Hydrogen absorption by a Pd film detected by microgravimetry1, J.J. Avila, R. Trabol, U.G. Volkmann, A.L. Cabrera, Pontificia Universidad Catolica de Chile, C. Romero, P. Lievens, Katholieke Universiteit Leuven — A thin film of palladium (200 Å) was e-beam evaporated onto a quartz crystal used in a SQM-160 Microbalance from Sigma Instruments. The crystal was then successively exposed to different hydrogen pressures, in situ, and the change in the resonant frequency was recorded as a function of time. Hydrogen absorption by the Pd film can be obtained by the shift of the resonant frequency upon hydrogenation at different pressures. A 14 Hz shift is obtained when the Pd film is saturated with hydrogen at 10 Torr of pressure. The different faces of the Pd-H system are observed with this technique.

5:18PM D12.00015 Observation of In Plane Magnetization Reversal Using Polarization Dependent Magnetooptical Kerr Effect, Hendrik Ohldag, Stanford Synchrotron Radiation Lightsource, Menlo Park, CA USA, Franz Hillebrecht, Institute for Solid State Research, Juelich Germany — We present an experimental setup for in plane two axis magnetometry by employing the polarization dependence of the magnetooptical Kerr effect. (MOKE). The proposed approach allows for observing the complete in plane reversal process during a hysteresis loop. For this purpose a conventional setup to measure longitudinal MOKE with crossed polarizers is extended by a Faraday cell to compensate for the rotation of the polarization vector caused by the magnetized sample. This detection scheme enables us to observe hysteresis loops of single monolayer. Using a Jones matrix formalism we are able derive expressions for the Kerr rotation using oblique incident polarization, allowing for extracting 2-dimensional vectorial information about the magnetization reversal process in the plane of the sample surface. The approach can be further extended to extract all three components of the magnetization by acquiring more than two loops. Since this setup does not require to change the sample geometry in situ it can be easily attached to an existing ultra high vacuum setup.

Monday, March 16, 2009 2:30PM - 5:30PM  
Session D13 SPS Undergraduate Research II 309

2:30PM D13.00001 SESSION BREAK –

2:42PM D13.00002 Phase measurements on a subwavelength optical metamaterial based on metallic paired strips1, Kara Maller, Thomas Jarvis, Xiaqiong Li, Dmitriy Korobkin, Gennady Shvets, Department of Physics, University of Texas at Austin, Austin TX 78712-0264, Marcelo Davanco, Xuhuai Zhang, Department of Physics, University of Michigan, Ann Arbor MI 48109-1040, Stephen R. Forrest, Department of Physics, Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor MI 48109-1040, — There is no known naturally occurring material with negative index of refraction because the electrical and magnetic resonances in naturally occurring materials do not overlap in frequency. However, artificially engineered materials, known as metamaterials, can be designed to exhibit such peculiar properties. We study a subwavelength optical metamaterial composed of paired gold strips separated by a continuous gold film. According to theoretical calculations, this structure is expected to display a negative index of refraction in the near-infrared. We perform phase measurements of the material using a polarization interferometer and a tunable femtosecond laser. The phase information of the transmitted wave at various wavelengths is used to characterize the index of refraction.

1Research is supported by NSF DMR-0747822.

2:54PM D13.00003 Undergraduate Research with Josephson Qubits: From Fabrication to Spectroscopy1, Alyssa Wilson, Jerome Mlack, Anthony Tyler, Zechariah Thraillkill, Joseph Lambert, Roberto Ramos, Drexel University — Josephson junctions are scalable solid state devices that can be used as qubits in quantum computing. In this talk we will describe the different stages involved in the fabrication, characterization and state measurement of a particular superconducting qubit known as the Josephson phase qubit. We have performed current-voltage measurements that determined the critical current of our device and produced histograms of switching currents that were needed to establish the quantum state of the junction. We will also report on the progress on microwave spectroscopy measurements involving multiple qubits coupled using on-chip capacitors. Spectroscopy reveals the various energy levels of entangled quantum states. We will discuss how physics undergraduates have contributed to this work.

1We would like to acknowledge the Wellstood Group at the University of Maryland for helpful discussions.
3:06 PM D13.00004 Degradation Studies of Polymer Blend Photovoltaics, BRIAN JOHNSON, ENAANE ALLAGOA, ROBERT THOMAS, GREG STETTLER, MARIANNE WALLIS, JUSTIN PEEL, BRIAN MCNELIS, RICHARD BARBER, Santa Clara University — We have measured the time dependence of device performance for photocells using blends containing the conjugated polymer, Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV) with different functionalized C60 electron acceptor molecules: commercially available [6,6]-Phenyl C61 butyric acid methyl ester (PCBM) or [6,6]-Phenyl C61 butyric acid octadecyl ester (PCBO) produced in our laboratory. Performance was characterized by the maximum power output of the devices, with the time dependence typically following an exponential decay. Variations in the characteristic lifetime of the devices were observed to depend on the molar fraction of the electron acceptor molecules (calculated with respect to the MEH-PPV monomer fraction). Differences in the decay behavior between the PCBM and PCBO blends will be presented.

1Supported by SCU Internal and Technology Grants

3:18 PM D13.00005 Coulomb Blockade I-V Characteristics in Nanowires, SARAH JOY, GUNDETA SINGHBHALLA, ARTHUR HEBARD, AMLAN BISWAS, SELMAN HERSHFIELD, University of Florida — The current-voltage (I-V) characteristics of manganite nanowires seen in an experiment closely resemble the hallmark I-V curves of the Coulomb blockade. Unlike normal Coulomb blockade curves, these curves have multiple lines instead of one, branching out from the zero current point. In order to discover an explanation for these I-V curves a simulation based on the Coulomb blockade was done for multiple junctions, because the experiments were done in a regime where multiple islands of ferromagnetic material are separated by insulating regions, as a result of intrinsic phase separation. The simulation results show I-V curves that are in good qualitative agreement with the experiment. The branching of I-V curves is due to a large change in resistance between the islands – not a change in the capacitance. Analytic work shows that the change in the junction resistance is too large to be explained by the tunneling magnetoresistance, but consistent with a change in the barrier thickness or composition. Simulations of the effect of gates show that the low voltage regime changes periodically with the gate voltage, while the high voltage regime is independent of gate voltage.

Supported by the U.F. Physics REU program

3:30 PM D13.00006 A quartz tuning fork as a force sensor for atomic force microscopy, ARTHUR IANUZZI, JULIA NEFF, JOHN TIMMERWILKE, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, FL 32611 — We are designing and building an atomic force microscope (AFM) to characterize the surface properties of perovskite oxides in low temperature (~10K) and high magnetic field (9T) environments. We are using a quartz tuning fork as the force sensor. The z-axis displacement of a conducting AFM tip due to surface features will be detected by observing the shift in resonance frequency of the tuning fork which is attached to the tip. The conducting tip will also allow us to perform conductive atomic force microscopy. The resonance characteristics of the tuning fork element were determined in various degrees of vacuum, with and without the tip installed, and as a function of the tip’s proximity to the sample surface. We show that the high resonance frequency (~32kHz) and quality factor (~30,000) of the tuning fork makes it an extremely sensitive force detector. The apparatus has also been designed with the capability of performing magnetic force microscopy on perovskite oxides.

Supported by NSF DMR-0804452

3:42 PM D13.00007 Mossbauer Study of the xCr2O3-(1-x)α-Fe2O3 nanoparticles system, SEAN KRUPA, MONICA SORESCU, Duquesne University — The xCr2O3-(1-x)α-Fe2O3 nanoparticles system was synthesized hydrothermally for x = 0.0 to x = 0.9. Mossbauer spectroscopy was performed on the obtained samples as well as for samples subjected to thermal annealing at 550°C for one hour. At x = 0.1, the as obtained samples began showing superparamagnetism and became completely superparamagnetic after x = 0.4 concentration. The percent of the sample that was superparamagnetic increased with Cr2O3 substitution. This correlates with chromium decreasing the particle size of the powder. The thermally annealed samples appeared to have the hematite structure re-grown for concentrations x = 0.1 to x = 0.4 with the intensity of the hyperfine magnetic field decreasing with Cr2O3 concentration. For x = 0.5 to x = 0.9, the percent of superparamagnetic particles increased with Cr2O3 concentration, dominating the system by x = 0.8. This system is believed to have applications in gas sensing and catalysis.

3:54 PM D13.00008 Construction of a semiconductor laser system for magneto-optical trapping of atomic rubidium, J. AN DOUGHERTY, MICHAEL LIM, Dept. of Physics, Rowan University — We report on the construction of a semiconductor laser system to generate light for magneto-optical trapping of rubidium. A DFB laser is used as a master oscillator with rapid frequency tuning accomplished by an acousto-optic modulator in double-pass configuration. The resulting beam seeds a 0.5-W tapered semiconductor amplifier chip. We spatially mode-match the output to a polarization-maintaining, single-mode fiber using lenses and two anamorphic prism pairs. At maximum efficiency the system generates more than 100 mW of TEM00 power at the fiber output.

Supported by NSF PHY-0613659, Research Corporation C66180, and the Rowan College of Liberal Arts and Sciences

4:06 PM D13.00009 Combinatorial Synthesis of (V1−x,Crx)4GeC3 Epitaxial Films, C. E. STEINMETZ, J. R. APPLLEGATE, S. M. BENJAMIN, B. D. ADAMSON, J. D. HETTINGER, S. E. LOFLAND, Department of Physics and Astronomy, Rowan University, T. H. SCABAROZI, Department of Materials Science and Engineering, Drexel University — We report the synthesis of solid solutions of (V1−x,Crx)4GeC3 epitaxial films on single crystal Al2O3 epi-polished substrates. The materials are sputtered from four cathodes; three are powered by rf-power supplies while one is driven by a dc-power supply. The materials are co-deposited at a temperature of 900°C and we get solubility across the whole range of compositions. The substrate-film interaction creates a strain which makes the new phase energetically favorable. The surface structure was measured using atomic force microscopy revealing that the composition has little impact on this property. We found a new MAX-phase material, (V0.5Crx0.5)4GeC3, which has never been synthesized in bulk form. We report the conditions required to make these materials. In addition, electrical transport characteristics as a function of composition will be reported.

This work supported by the National Science Foundation through DMR-0503711.

4:18 PM D13.000010 ABSTRACT WITHDRAWN —
4:30PM D13.00011 Thermodynamic Properties of Ising Spins on the Triangular Kagomé Lattice
BILIN ZHUANG, COURTNEY LANNERT, Wellesley College, Wellesley, MA 02481 — The triangular Kagomé lattice can be constructed by inserting a lattice site on each bond of the Kagomé lattice. Each unit cell contains 6 α-sites, 3 β-sites, 6 aa-bonds and 12 ab-bonds. The lattice with antiferromagnetic aa-bonds is known to exhibit geometrical frustration at low temperatures. We applied analytical methods and Monte Carlo simulations to study a system of Ising Spins on the lattice and investigated its thermodynamic properties. In particular, the heat capacity of the model exhibits interesting features based on the strength and the sign of coupling constants \( J_{ab} \) and \( J_{aa} \). In the case when the aa-interaction is antiferromagnetic, the heat capacity shows two broad peaks at \( kT/J_{ab} \approx 1.8 \) and at \( kT/J_{aa} \approx 1.8 \). In the case when the aa-interaction is ferromagnetic, the heat capacity shows a sharp peak at \( kT/J_{ab} \approx 1.9 \) and another low broad peak at around \( kT/J_{aa} \approx 1.4 \). We also studied a much simpler system of two α-trimers connected with β-sites to reproduce the thermodynamics behaviors of the more complicated triangular Kagomé lattice and to further understand the origin of its interesting properties.

1Supported by Jerome A. Schiff Fellowship

4:42PM D13.00012 Monte Carlo Simulations of a 111-Ising Dipolar Model on the Hyper-
kagomé Lattice
PATRICK CARTER, Department of Physics Southern CT State University New Haven, CT, JOHN HOPKINSON, Department of Physics & Astronomy Brandon University Brandon, Manitoba, Canada, MATTHEW ENJALRAN, Department of Physics Southern CT State University New Haven, CT — Motivated by the physics of dipolar spin ice, we investigate the hyper-kagomé lattice with 111-Ising spins. The hyper-kagomé lattice can be generated by a selective removal of one site per tetrahedron of the pyrochlore lattice to yield a lattice of corner-sharing triangles. The spin-1/2 ions of Na\(_{11}\)O\(_8\) represent an experimental realization of the hyper-kagomé structure. We report preliminary results from Monte Carlo simulations of the 111-Ising dipolar hyper-kagomé model, which represents a yet to be studied disorder-free limiting case of diluted spin ice.

1Work supported by a Cottrell College Science Award, Research Corporation (ME and PC) and NSERC of Canada (JMH).

4:54PM D13.00013 Thermal measurements of the MAX-phase material Cr\(_2\)GeC\(_1\)
D. T. PIWOWAR, P. ABBAZIA, D. FILOMENA, D. DOROFY, M. GARZON, S. E. LOFLAND, J. D. HETTINGER, Department of Physics and Astronomy, Rowan University, T. H. SCABAROZI, Department of Materials Science and Engineering, Drexel University — We have measured the specific heat and thermal transport in bulk Cr\(_2\)GeC\(_1\) samples that have been hot-isostatically-pressed or hot pressed. We observe no difference in the results based upon the synthesis procedure. We find the low temperature specific heat is fit well by the standard expression. These measurements suggest a large density of states at the Fermi level or a large electron-phonon coupling in this material. The Debye temperature, extracted from the phonon contribution to the specific heat, is found to be 460 K, which roughly correlates with the Debye temperature extracted from the ultrasonic elastic measurements. The phonon contribution to the thermal conductivity will also be reported.

1This work supported by the NSF through grant DMR-0503711.

5:06PM D13.00014 ABSTRACT WITHDRAWN —

5:18PM D13.00015 Borosilicate films as permeability barriers
J. R. APPLEGATE, C. E. STEINMETZ, J. D. HETTINGER, Department of Physics and Astronomy, Rowan University, J. F. CARROLL, R. KRCHNAVEK, Department of Electrical and Computer Engineering, Rowan University — Borosilicate films have been deposited using rf-sputtering techniques from a composite target at room temperature onto polypropylene (PP), high density polyethylene(HDPE), low density polyethylene(LDPE), and polyethylene terephthalate (PETG) substrates. Films were found to be smooth, flexible, with excellent adhesion to the substrates. Repeated rolling the coated substrates on a radius of 0.5mm resulted in no discernable damage for films less than 200nm in thickness. Creasing the substrates did result in local damage. However excellent adhesion did not allow the fractured glass to come off the substrate. Heat generated during deposition only influenced the films grown on LDPE where the thermal expansion mismatch between the film and substrate induced strains caused fractures in thick films. Modifications to processing parameters allowed thick films to be grown without fractures. Permeability measurements of nitrogen resulted in significant improvements in comparison to uncoated substrates.

1This work supported by Wheaton Industries, Inc. Millville, NJ

Monday, March 16, 2009 2:30PM - 5:30PM — Session D14 DFD: Colloids II: Structure and Rheology 315

2:30PM D14.00001 Lock and Key Colloids
STEFANO SACANNA, WILLIAM IRVINE, PAUL CHAIKIN, DAVID PINE, NYU — We demonstrate a recognition mechanism between microscopic (colloidal) particles based on a simple “lock-and-key” principle that relies only on the complementary morphology of the particles involved. The system we developed consists of charge-stabilized spherical silica colloids (keys) and specially designed polymeric particles with spherical cavities (locks). The assembly of locks with keys is driven by depletion interactions between the particles and an uncharged water-soluble polymer (poly-ethylene oxide). We show that by balancing electrostatic repulsion and depletion attraction, we induce a selective and reversible lock-and-key self-assembly. Moreover, we can design the lock and key single units to have separate functionalizable chemistries, such that the resulting composite particle (lock+key) will exhibit anisotropic surface properties.

1This work was supported by The Netherlands Organisation for Scientific Research (NWO).

2:42PM D14.00002 ABSTRACT WITHDRAWN —

2:54PM D14.00003 Pairwise Additivity in Colloidal Electrostatics
JASON W. MERRILL, Yale University, SUNIL K. SAINIS, Rowland Institute, ERIC R. DUFRESNE, Yale University — We present a method for measuring electrostatic and hydrodynamic interactions between colloidal particles based on observations of short-time trajectories. We use this method to explore whether forces between colloidal particles can be considered pairwise additive by comparing the force between a pair of particles to forces between groups of several particles.
3:06PM D14.00004 Structure and dynamics of suspensions of nanoparticles in nematic liquid crystals. BRIAN GETTELFINGER, GARY KOENIG, JOSE MORENO-RAZO, University of Wisconsin, JUAN HERNANDEZ-ORTIZ, Universidad Nacional de Colombia, NICHOLAS ABBOTT, JUAN DE PABLO, University of Wisconsin — A hierarchical modeling approach has been adopted to examine the structure and dynamics of nanoparticles suspended in liquid crystals. A molecular model is used to predict the defects that arise in nanoparticle assemblies, as well as their response to applied flow fields. The model is solved by resorting to a radial basis function based technique. The validity of the model and our numerical results are established by direct comparison to results from molecular dynamics simulations of nanoparticles in nematic and isotropic liquid crystals. Results for particle diffusion and aggregation at equilibrium and in flowing systems are then used to interpret our experimental data for a variety of systems.

3:18PM D14.00005 Monodisperse polymethyl methacrylate (PMMA) spheres in organic media: synthesis update, ANDREW HOLLINGSWORTH, MARK ELSesser, WILLIAM IRVINE, DAVID PINE, PAUL CHAIKIN, New York University — Since the publication of Antl, et al. [Colloids and Surfaces 17 (1986) 67–78] more than 20 years ago, several research groups in the soft condensed matter area have attempted the dispersion polymerization of sterically-stabilized PMMA particles. Most have found that success of this particular synthesis depends critically on the quality of the comb-graft stabilizer, poly(12-hydroxystearic acid)-g-PMMA. More recent work has extended the particle synthesis to include the incorporation of covalently attached, fluorescent dyes in the particle interior. Our goal has been to reproduce some of these results—a challenging task—and to improve the process, leading to a reliable method for preparing core-dyed PMMA particles. We will report on several important findings related to this research goal, and demonstrate that our particles can be used to make colloidal clusters via the recently published emulsion encapsulation and shrinkage technique [Science 301, 483–487 (2003)].

3:30PM D14.00006 A model nanocolloidal rod system to explore structural transitions in networks and bundles, GEORGINA WILKINS, University of Michigan, PATRICK SPICER, The Procter and Gamble Company, MICHAEL SOLOMON, University of Michigan — We introduce a model system consisting of self-assembled polyamide anisotropic colloids suspended in aqueous surfactant solutions. The colloidal particles are formed by precipitation from an amorphous polyamide powder that is dispersed with mechanical agitation in an aqueous surfactant phase at temperatures from 59 to 100 °C. The aspect ratio increases monotonically with temperature; at T = 50°C, short rods with aspect ratio r = 8 ± 1 form. At T = 100°C, rope like structures with r = 306 ± 14 form. By confocal laser scanning microscopy (CLSM) and dynamic light scattering (DLS) as volume fraction is increased we show a structural transition from dilute rod behaviour with diffusive dynamics to a homogeneous network structure with increasing slow dynamics. Furthermore, increasing the aspect ratio of rods induces the same structural transition from dilute rod behaviour to a network structure. Finally, we vary the interaction potential between the rods by a polymer induced depletion interaction and observe an unexpected quiescent network to bundle transition. The bundles are several rod diameters wide and 1 - 2 rod lengths long. The rods appear to order naturally within each bundle. The bundling transition leads to an order of magnitude decrease in the storage modulus of the suspensions.

3:42PM D14.00007 Polymer grafted particles: Architectural effects on the dynamics, PANAYIOTIS VOUDOURIS, F.O.R.T.H., Heraklion, Greece, JIHOON CHOI, HONG DONG, Carnegie Mellon University, Pittsburgh, USA, GEORGE FYTAS, F.O.R.T.H., Heraklion, Greece, MICHAEL BOCKSTÄLLER, KRIS MATYJASZEWSKI, Carnegie Mellon University, Pittsburgh, USA — We present a combined static and dynamic light scattering study of two polystyrene particles with different grafting densities. The particle solution systems in which tuning of the grafting density and molecular weight of the surface bound PS afford intermediate (0.5nm−2) and concentrated (0.94nm−2) brush densities. The different packing environment of PS chains give rise to distinctly different rich dynamic response above a threshold volume fraction that yields insight into the role of polymer grafts on the structure formation of hairy particles. This work is the first report on the mixing dynamics of hybrid core-shell nanoparticles with distinct behavior intermediate between ultra soft multiarm star polymers and hard sphere colloids. With increasing grafting density of PS ligands the dynamic properties approach those of hard sphere systems while retaining some of the polymer-specific dynamic characteristics.

3:54PM D14.00008 Structure of Quasi-One Dimensional Ribbon Colloid Suspensions1, BINHUA LIN, STUART A. RICE, The University of Chicago, THOMAS STRATOS, BIANXIAO CUI, Stanford University — We report the results of an experimental study of a colloid fluid confined to a quasi-one dimensional (q1D) ribbon channel. Our findings confirm the principal predictions of previous theoretical studies of such systems. These are (1) that the density distribution of the liquid transverse to the ribbon channel exhibits stratification and (2) that even at the highest density the order along the strata, as measured by the longitudinal pair correlation function, is characteristic of a liquid.

4:06PM D14.00009 Dynamics of Internal Stresses and Scaling of Strain Recovery in Aging Colloidal Gels, AJAY SINGH NEGI, CHINEDUM OSUJI, Department of Chemical Engineering, Yale University — On cessation of flow, dilute suspensions of carbon black particles undergo rapid gelation and display instantaneous residual or internal stresses which relax slowly with time. We monitor the evolution of these stresses (under zero strain) and find a weak power law decay, σi ~t−α over 5 decades of time where α ≈ 0.1. The system exhibits aging, with the elastic modulus scaling as a weak power law of elapsed time, G ∼ t−β, with β ≈ α. Imposition of zero stress conditions after waiting time tω, at internal stress σω (tω), results in strain recovery at the system relaxes without the zero strain constraint. Older systems exhibit less recovery than younger ones. Remarkably, strain recoveries at different tω can be shifted to construct a single master curve in which the magnitude of the recovery is shifted vertically according to σi(tω) = 1−tω and horizontally simply with elapsed time. The scaling of the strain recovery with internal stress suggests that the internal stress state is characteristic of the age of the system and of the manner in which the system will continue to evolve. This result has important implications for our understanding of glassy behavior in soft materials.

4:18PM D14.00010 Synthesis and Self-assembly of Janus and Patchy Particles by Lift-up Microcontact Printing, SHAN JIANG, STEVE GRANICK, University of Illinois at Urbana and Champaign — Janus and patchy particles were synthesized by a simple and novel lift-up microcontact printing method. The geometry of the particles is revealed by both optical fluorescence microscopy and scanning electron microscopy. It is demonstrated that the Janus balance (geometry) of the particles can be easily fine tuned. Interesting and unique cluster structures were self-assembled from particles synthesized by this method. The method allows particles not only of divalent but also of trivalent geometry to be formed in large quantity.

4:30PM D14.00011 Thermal Properties of Particulate Suspensions, REBECCA CHRISTIANSON, JESSICA TOWNSEND, Franklin W. Olin College of Engineering — It has been known since the 1800’s that additions of solid phase particles to a liquid can improve the thermal conductivity of the liquid. However, the instability of such suspensions makes the technique impractical for commercial applications. With the advent of affordable technology for synthesizing nanometer scale particles, it became possible for stable suspensions with improved thermal properties to be created. Initial investigations of nanoparticle suspension coolants (termed nanofluids) seemed to indicate an anomalous enhancement of the thermal conductivity above that predicted by conventional theories. However, subsequent experimental work showed issues with the reproducibility of these early results, which has been attributed by some sources to a tendency to aggregate due to the high nanoparticle suspensions, as well as our initial findings on the effects of aggregation on the measured thermal properties of particulate suspensions.
we here present an effective treatment of the intramolecular degrees of freedom of water, where these modes are decoupled from the intermolecular one, adiabatically allowing these coordinates to be positioned at their local minimum of the PES. This decoupling is performed combining an AIMC simulation using the rigid bodies approximation with an intramolecular optimization. As an application of our methodology we have studied small water clusters. We show that even in the case of the water dimer the sampling of phase space is significantly modified when intramolecular optimization is included (J. Chem. Phys., 128, 104311 (2008)). As a result, there are clear changes in features such as the dipole moment and structural properties.

Related publications:

1We acknowledge financial support from FAPESP and CNPq.

5:06PM D14.00014 New look of fractional exclusion statistics1, DRAGOS-VICTOR ANGHEL, Department of Theoretical Physics, Horia Hulubei National Institute of Physics and Nuclear Engineering — I discuss the concept of fractional exclusion statistics and I show that it leads to inconsistencies in the calculation of the particle distribution that maximizes the partition function. These inconsistencies appear when mutual exclusion statistics is manifested between different subspecies of particles in the system. In order to eliminate these inconsistencies, I introduce new mutual exclusion statistics parameters, which are proportional to the dimension of the Hilbert sub-spaces on which they act. These new definitions lead to properly defined particle distributions and thermodynamic properties. I also show that fractional exclusion statistics is manifested in general interacting systems and I calculate the exclusion statistics parameters. Most importantly, I prove that indeed, the mutual exclusion statistics parameters are proportional to the dimension of the Hilbert space on which they act.

Related publications:

1Partially supported by NATO EAP.RIG 982080.

5:18PM D14.00015 Capillary forces on nanowires, JUN MA, SHENFENG CHENG, Johns Hopkins University, JAY WALLACE, MACS Consulting, PATRICIA MCCUIGAN, MARK ROBBINS, Johns Hopkins University — The capillary forces on nanowires have been measured by attaching them to the cantilever of an Atomic Force Microscope (AFM). The nanowires are immersed and retracted from a liquid/air interface. The entire capillary force curve is compared to continuum theory and molecular simulations. Nanowires with different diameters and chemistry and various liquids are investigated. Surface tension, contact angle hysteresis, and dynamical contact angles can be extracted under reasonable assumptions about how the contact line moves along the nanowires.
3:18PM D15.00005 Large-scale free-standing monolayer membranes of nanoparticles: preparation and properties. JINBO HE, LASZLO FRAZER, James Franck Institute, University of Chicago, Chicago, Illinois 60637, USA, XIAO-MIN LIN, Materials Science Division, Chemistry Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA, ADAM WEIS, HEINRICH JAEGER, James Franck Institute, University of Chicago, Chicago, Illinois 60637, USA — Two-dimensional arrays of close-packed nanoparticles can be stretched across tens-micrometre-size holes. The resulting freestanding monolayer membranes extend over hundreds of particle diameters without cross-linking of the ligands or further embedding in polymer. In our previous results of dodecanethiol-ligated 6-nm-diameter gold nanocrystal monolayers, we find a Young’s modulus of the order of several GPa. This remarkable strength is coupled with high flexibility, enabling the membranes to bend easily while draping over edges. Recently we found that oleic-acid-covered cobalt nanoparticles (~9 nm in diameter) self-assemble at toluene/ethylene glycol interfaces and form large two-dimensional arrays. These membranes stretch across tens-of-micrometer holes after drying of ethylene glycol. The mechanical and diffusion properties of these membranes are tested and the response of these membranes under external fields is also investigated.

3:30PM D15.00006 Casimir force between inclusions in a stretchable fluid membrane, HSUANG-KU LIN, ROYA ZANDI, LEONID PRYADKO, Department of Physics, University of California at Riverside — We calculate the entropic fluctuational force, a finite-temperature analogue of the Casimir force, between foreign inclusions in a stretchable fluid membrane. Specifically, we consider the fluctuations of a planar membrane governed by the full Helfrich Hamiltonian, including the surface tension and both bending rigidity terms. The inclusions are introduced as circular regions where the surface tension and/or bending rigidities are modified from their values on the non-perturbed membrane. Results for arbitrarily-strong perturbations of the membrane, including holes, rigid disks, and edges will be presented.

3:42PM D15.00007 Breathable NIPAAm Network with Controllable Hydration Supports Model Lipid Membrane, MICHAEL JABLIN, HILARY SMITH, MIKHAIL ZHERNENKOV, Lujan Neutron Scattering Center, AJAY VIDYASAGAR, RYAN TOOMEY, University of South Florida, JESSICA SAIZ, Lujan Neutron Scattering Center, BORIS TOPERVERG, Ruhr Universitat Bochum, ERIK WATKINS, TONYA KUHL, University of California, Davis, ALAN HURD, JAROSLAW MAJEWSKI, Lujan Neutron Scattering Center — The interaction of a model lipid bilayer composed of DPPC with a surface-tethered poly(N-isopropylacrylamide) (NIPAAm) was explored with neutron reflectometry (NR). The Langmuir-Blodgett / Langmuir-Schaeffer method was used to deposit a lipid bilayer onto the polymer. NR measurements were used to probe the in- and out-of-plane structure of the system as a function of temperature. NR with fluorescence microscopy show that the polymer supports a lipid bilayer and hydration of the support can be controlled. At low temp., the membrane develops out-of-plane undulations visible in off-specular scattering. Analysis of the off-specular reveals in-plane correlation of the bilayer fluctuations. The separation of the lipid bilayer from the solid support of a substrate constitutes a significant step towards a more realistic model of biological membranes.

3:54PM D15.00008 The effects of lung surfactant peptide mimic KL4 on lipid monolayer collapse, NIELS HOLTEN-ANDERSEN, University of Chicago, Department of Chemistry, Chicago, IL 60637, USA, LUKA POCIKAVICEK, University of Chicago, Department of Chemistry and James Franck Institute, Chicago, IL 60637, USA, ALAN J. WARING, University of California, Los Angeles, School of Medicine, Department of Medicine, Los Angeles, CA 90095, USA, KA YEE C. LEE, University of Chicago, Department of Chemistry and James Franck Institute, Chicago, IL 60637, USA — We have investigated the origin of the positive effect of the peptide KL4 on lung surfactant lipid monolayers containing DPPC and POPG. Using surface balance techniques and fluorescence microscopy we have observed that KL4 rigidifies POPG containing lipid monolayers evidenced by a shift in their collapse mode. Rather than collapsing as a fluid by flowing into the sub-phase, a KL4 supported POPG monolayer instead collapses by folding. Furthermore, when KL4 is added to POPG containing monolayers they demonstrate an increased tolerance to repeated compression and expansion cycles while the opposite appears to be true for pure DPPC monolayers. We will discuss the potential role of electrostatic interactions in the rigidifying effect of KL4 on POPG containing monolayers in the context of the overall importance of collapse mode in establishing robust and reversible lipid monolayers.

4:06PM D15.00009 Microrheology of protein layers at the air-water interface, MYUNG HAN LEE, STEVEN CARDINALI, DANIEL REICH, Johns Hopkins University, KATHLEEN STEBE, University of Pennsylvania, ROBERT LEHENY, Johns Hopkins University — Due to their amphiphilic nature, many proteins in aqueous solution will adsorb at the air-water interface to create a viscoelastic interfacial layer. We present an investigation of the formation and mechanical properties of interfacial protein layers formed by beta-lactoglobulin using microrheological techniques including multiple particle tracking and magnetic nanowire microrheology. We observe the interfacial rheology evolve in time through three stages: (i) an increase in viscosity, (ii) a period of spatial heterogeneity in which the interface contains elastic and viscous regions, and (iii) the development of a uniformly rigid elastic film. We evaluate the dependence of this evolution on the protein-protein interactions, which we tune by varying solution pH. As we will discuss, these studies illustrate the power of microrheological approaches to interfacial rheology.

4:18PM D15.00010 ABSTRACT WITHDRAWN

4:30PM D15.00011 Critical swelling of fluctuating capsules, FABRICE THALMANN, University of Strasbourg and Institut Charles Sadron CNRS, CARLOS M. MARQUES, Institut Charles Sadron CNRS and University of Strasbourg — We consider a single polymer chain, grafted on a flat and rigid substrate, covered by a membrane. The membrane presents some affinity for the surface, caused by non specific adhesive interactions. The challenge is to anticipate and describe the different possible relative configurations of the membrane and the polymer chain, depending on parameters such as the surface tension and curvature of the membrane, or the chain gyration radius. We propose for this system a phase diagram of the different regimes, as well as quantitative predictions for comparison with some recent experiments.

4:42PM D15.00012 Monday, March 16, 2009 2:30PM - 5:30PM — Session D16 DAMOP: Focus Session: BEC-BCS Crossover

Critical swelling of fluctuating capsules, HAIM DIAMANT, EMMIR HALEVA, Tel Aviv University — In many natural transport processes the solute molecules to be transported are encapsulated in semipermeable, flexible membrane vesicles of micron size. We study the swelling of such fluctuating capsules, as the number of encapsulated particles is increased, or the concentration of the outer solution is decreased. The approach to the maximum volume-to-area ratio and the associated buildup of membrane tension involve a continuous phase transition and follow universal scaling laws. The criticality and its features are model-independent, arising solely from the interplay between volume and surface degrees of freedom.

2:30PM D16.00001 BCS to BEC evolution for mixtures of fermions with unequal masses\(^1\). CARLOS A. R. SA DE MELO, Georgia Institute of Technology — I discuss the zero and finite temperature phase diagrams of a mixture of fermions with unequal masses with and without population imbalance, which may correspond for example to mixtures of \(^6\)Li and \(^40\)K, \(^6\)Li and \(^87\)Sr, or \(^40\)K and \(^87\)Sr in the context of ultracold atoms. At zero temperature and when excess fermions are present, at least three phases may occur as the interaction parameter is changed from the BCS to the BEC regime. These phases correspond to normal, phase separation, or superfluid with coexistence between paired and excess fermions. The zero temperature phase diagram of population imbalance versus interaction parameter presents a remarkable asymmetry between the cases involving excess lighter or heavier fermions [1, 2], in sharp contrast with the symmetric phase diagram corresponding to the case of equal masses. At finite temperatures, the phase separation region of the phase diagram competes with superfluid regions possessing gapless elementary excitations \([3]\) for certain ranges of the interaction parameter depending on the mass ratio. Furthermore, a phase transition may take place between two superfluid phases which are topologically distinct. The precise location of such transition is sensitive to the mass ratio between the two species of fermions. Signatures of this possible topological transition are present in the momentum distribution or structure factor, which may be measured experimentally in time-of-flight or through Bragg scattering, respectively. Lastly, throughout the evolution from BCS to BEC, I discuss the critical current and sound velocity for unequal mass systems as a function of interaction parameter and mass ratio. These quantities may also be measured via the same techniques already used in mixtures of fermions with equal masses.


\(^1\)Work supported by NSF (DMR-0709584).

3:06PM D16.00002 Spin-imbalanced atomic Fermi gases in one dimension and the prospects for FFLO superconductivity\(^1\). C.J. BOLECH, P. KAKASHVILI, Rice University — Growing expertise to engineer, manipulate and probe different analogs of condensed matter systems allows to probe properties of exotic pairing states such as the Fulde-Ferrell-Larkin-Ovchinnikov state. Inspired by ongoing experiments at Rice university, we are studying the pairing in spin-imbalanced ultracold atomic system of fermions in one dimension. Calculations are done using the Bethe Ansatz technique and the trap is incorporated into the solution via local density (Thomas-Fermi) approximation. The thermodynamic-Bethe-Ansatz equations are solved numerically and different density profiles (total-, spin- and entropy-densities) are calculated in the trap for different finite temperatures. A scheme to identify the phase diagram using total density profiles in the trap is proposed that would be immediately useful for experimentalists.

3:18PM D16.00003 Finite temperature effects of \(^6\)Li-\(^40\)K mixtures in the BCS-BEC crossover, HAO GUO, CHIHCHUN CHIEN, YAN HE, Univ. of Chicago, QIJIN CHEN, Zhejiang Univ., KATHRYN LEVIN, Univ. of Chicago — Recent experiments on mixtures of ultra-cold fermions of different species inspire study of pairing between fermions with different masses. We study systematically \(^6\)Li-\(^40\)K mixtures with tunable attractive interactions in the BCS-Bose Einstein condensation crossover. Pairing fluctuations which are important at finite temperatures are included in a consistent fashion. Population imbalance of the two species is also considered. We found an intermediate-temperature superfluid phase which is similar to the one found in polarized Fermi gases with equal mass. We present superfluid transition temperature for a broad range of polarization and interaction strength and analyze stability of possible superfluid phases. Phase diagrams at and near unitarity are presented. Polarized superfluids are shown to be stabilized when the light species is the majority. Thus, in contrast to pairing between fermions with equal mass, observation of stable low-temperature polarized superfluids near unitarity is more feasible in \(^6\)Li-\(^40\)K mixtures.

3:30PM D16.00004 Phenomenology Of Trapped Polarized Fermi Gases, LESLIE BAKSMATY, Rice University, HONG LU, Rice University, HAN PU, CARLOS BOLECH, Rice University — We discuss recent, apparently contradictory experimental results on trapped, polarized, resonantly interacting interacting fermions. Our analysis occurs in the context of a full 3D Bogoliubov-de Gennes analysis and we dwell on the possible roles of the confining geometry in producing density distortions away from the local density approximation with implications for the Superfluid-Normal transition (Clogston limit).

3:42PM D16.00005 Rotation induced superfluid-normal phase separation in trapped Fermi gases, MENDERES ISKIN, EITE TIESINGA, Joint Quantum Institute (UMd and NIST) — We use the Bogoliubov-de Gennes formalism to analyze the effects of rotation on the ground state phases of harmonically trapped Fermi gases, under the assumption that quantized vortices are not excited. We find that the rotation breaks Cooper pairs that are located near the trap edge, and that this leads to a phase separation between the nonrotating superfluid (fully paired) atoms located around the trap center and the rigidly rotating normal (nonpaired) atoms located towards the trap edge, with a coexistence (partially paired) region in between. Furthermore, we show that the rotation reveals a topological quantum phase transition: the superfluid phase that occurs in the coexistence region is characterized by a gapless excitation spectrum, and that it is distinct from the gapped phase that occurs near the trap center.

3:54PM D16.00006 Pairing Instability in Two-Dimensional Rotating Fermion Liquids Near Unitarity\(^1\), PREDRAG NIKOLIC, Rice University — Fermionic superfluids can undergo phase transitions into different kinds of normal regimes, characterized by whether the Cooper pairs remain locally stable. If the normal phase retains strong pairing fluctuations, it behaves like a liquid of vortices as seen in cuprate superconductors. We argue that analogous strongly correlated normal states exist in two-dimensional neutral fermion liquids near unitarity, where superfluid is destroyed by fast rotation. The formal analysis is based on a model with SP(2N) symmetry which describes the quantum critical region in the vicinity of a broad Feshbach resonance. Assuming that pairing is the only instability in perturbation theory, we map the universal phase diagram in two-dimensions. Such a pairing instability is driven by macroscopically degenerate collective modes, which makes the Abrikosov flux lattice of the superfluid particularly susceptible to quantum melting. Combining this observation with a renormalization group analysis, we conclude that the unconventional normal states can be expected in the vicinity of the universal pairing instability, especially at low temperatures in the BCS limit.

\(^1\)Funded by W. M. Keck Program in Quantum Materials

4:06PM D16.00007 Number of closed-channel molecules in the BEC-BCS crossover, FELIX WERNER, University of Massachusetts, LETICIA TARRUELL, ETH Zurich, YVAN CASTIN, Ecole Normale Superieure — Using a two-channel model, we show that the number of closed-channel molecules in a two-component Fermi gas close to a Feshbach resonance is directly related to the derivative of the energy of the gas with respect to the inverse scattering length. We extract this quantity from the fixed-node Monte Carlo equation of state and we compare to the number of closed-channel molecules measured in the Rice experiment with lithium [Partridge et al., Phys. Rev. Lett. 95, 020404 (2005)].
in the weak coupling BCS limit, we find that the excitation of the breathing mode frequencies make the atomic cloud unstable. The critical anharmonicity depends on both rotational frequency and the chemical potential. As a result of the large chemical potential in the BCS regime, even with a weak anharmonicity the lowest order mode frequency decreases with increasing the attractive interaction. For large enough anharmonicities in the weak coupling BCS limit, we find that the excitation of the breathing mode frequencies make the atomic cloud unstable.

1Support: European Community (contract MEIF-CT-2006-041390), Dutch Foundation FOM, IFRAF Institute, ANR (grants 05-BLAN-0205 and 06-NANO-014-01), QUEDIS program of ESF, Austrian Science Foundation FWF, Russian Foundation for Fundamental Research.

4:42PM D16.00010 Two-fluid hydrodynamic modes in a strongly interacting Fermi gas1 . EDWARD TAYLOR, University of Trento, HUI HU, XIA-JI LIU, University of Queensland, SANDRO STRINGARI, University of Trento, ALLAN GRIFFIN, University of Toronto — Landau’s theory of two-fluid hydrodynamics provides an exact description of the low-energy dynamics of all strongly interacting superfluids described by a 2-component order parameter. Extending our recent work, we report on improved variational solutions of the two-fluid hydrodynamic modes in trapped two-component Fermi gases close to unitarity. We show that the two-fluid mode frequencies are identical to the predictions of regular (Euler) hydrodynamics except at certain temperatures where these in-phase modes strongly hybridize with out-of-phase modes. Although two-fluid hydrodynamic modes have been extensively studied in superfluid helium, experiments in trapped quantum gases have yet to detect a clear signal of these modes. We discuss the reasons for this and suggest several experimental signatures of two-fluid behaviour in trapped Fermi superfluids. Measuring the two-fluid mode frequencies is a promising way of testing microscopic theories of the thermodynamic and transport properties at unitarity.

4:54PM D16.00011 Adiabatic Dynamics of the Superconducting Order Parameter, MINXI JIANG, QIAN NIU, Department of Physics, The University of Texas, Austin, Texas — From the time-dependent variational principle and taking into Berry phase effects, we formulate the dynamics of superconducting order parameter in the region where it evolves much slower compared to the timescale of quasi-particles. Collective mode in this region is calculated and compared with previous result obtained from the random-phase approximation which is valid in the opposite limit. We discuss applications to BCS/BEC states of the quantum Fermi gases.

5:06PM D16.00012 The Efimov Effect and Color Superconductivity in a Three-State Fermi Gas . J.R. WILLIAMS, J.H. HUCKANS, E.L. HAZLETT, R.W. STITES, Y. ZHANG, K.M. O’HARA, The Pennsylvania State University — We have created a quantum degenerate $^4$Li gas with equal populations in the three lowest energy hyperfine states. This three-state Fermi gas is stable against two-body inelastic collisions but decays by three-body recombination. We measure the rate of three-body recombination which can be used as a signature of the Efimov effect and which determines whether conditions are favorable for BCS pairing. The three pairwise $s$-wave scattering lengths exhibit overlapping Feshbach resonances at 690, 810 and 834 Gauss. As we vary the field between 0 and 834 Gauss, we find that the three-body recombination rate constant varies by over four orders of magnitude. High stability is achieved near 0 and 570 Gauss. We observe narrow resonant loss features near 130 and 500 Gauss. Recent calculations indicate that these resonant features arise from Efimov trimer states near threshold[1]. We also report on the rate of three-body recombination between 834 and 2000 Gauss. Our determination of the three-body parameters in this regime will guide future experiments aimed at achieving color superconductivity in this system. E. Braaten, H.-W. Hammer, D. Kang, and L. Platter, arXiv:0806.0587.

5:16PM D16.00013 Phase diagram, extended domain walls, and soft collective modes in a three-component fermionic superfluid, GIANLUIGI CATELANI, EMIL YUZBASHYAN, Rutgers University — We study the phase diagram of a three-component Fermi gas with weak attractive interactions, which shows three superfluid and one normal phases. At weak symmetry breaking between the components the existence of domain walls interpolating between two superfluids introduces a new length scale much larger than the coherence length of each superfluid. This, in particular, limits the applicability of the local density approximation in the trapped case, which we also discuss. In the same regime the system hosts soft collective modes with a mass much smaller than the energy gaps of individual superfluids. We derive their dispersion relations at zero and finite temperatures and demonstrate that their presence leads to a significant enhancement of fluctuations near the superfluid-normal transitions.

Monday, March 16, 2009 2:30PM - 5:30PM — Session D17 GQI: Focus Session: Foundations of Quantum Theory 318

2:30PM D17.00001 LeRoy Apker Award Talk: Factoring Quantum Logic Gates with Cartan Involutions , BYRON C. DRURY, Haverford College — This abstract not available.
3:06PM D17.00002 Types and location of information¹, LOOI SHIANG YONG, VLAD GHEORGHIU, ROBERT B. GRIFFITHS, Carnegie Mellon University — Imagine having some quantum information encoded in \( n \) carrier qubits. We are interested in the question of how much information is present in a subset of the carrier qubits. In the case where the encoding is done using a stabilizer code, we have a precise and complete answer. The two extreme cases of having too small a subset whereby no information is present versus having a large subset of almost \( n \) qubits from which all the information can be extracted are already well understood. In this talk we focus on the intermediate situation where only partial information is present. For this purpose we define different “types” of information, where the presence of a type of information on a subset of carrier qubits implies the ability to distinguish a particular set of encoded states associated to that type. With this we can determine how much and what types of information are present in any given subset of carrier qubits. With the help of some simple examples, we will show how sometimes only “classical” information is present and sometimes more can be present. Finally our results can be generalized to higher dimensional qudit stabilizer codes.

¹The research described here received support from the National Science Foundation through Grants No. PHY-0456951 and PHY-0757251.

3:18PM D17.00003 Testing Born’s rule in Quantum Mechanics using a Triple slit experiment , URBASI SINHA, Institute for Quantum Computing (iQc), University of Waterloo, Canada, CHRISTOPHE COUTEAU, ZACHARI MESENDORP, IQC, Waterloo, Canada, IMMO SOELLNER, Institut fuer Experimentalphysik, Innsbruck, Austria, RAYMOND LAFLAMME, IQC, Waterloo, Canada, RAFAEL SORKIN, Syracuse University, Syracuse, NY, GREGOR WEHNS, Institut fuer Experimentalphysik, Innsbruck, Austria — In Mod. Phys. Lett.A 9 3119 (1994), one of us (R.D.S) investigated a formulation of quantum mechanics as a generalized measure theory. Quantum mechanics computes probabilities from the absolute squares of complex amplitudes, and the resulting interference violates the (Kolmogorov) sum rule expressing the additivity of probabilities of mutually exclusive events. However, there is a higher order sum rule that quantum mechanics does obey, involving the probabilities of three mutually exclusive possibilities. We could imagine a yet more general theory by assuming that it violates the next higher sum rule. In this presentation, we report results from an ongoing experiment that sets out to test the validity of this second sum rule by measuring the interference patterns produced by three slits and all the possible combinations of those slits being open or closed. We use either attenuated laser light or a heralded single photon source (using parametric down conversion) combined with single photon counting to confirm the single photon character of the measured light.

3:30PM D17.00004 Cartan Involutions in Quantum Information, PETER LOVE, Haverford College — We discuss some applications of Cartan decompositions and the corresponding involutions of the unitary group in quantum information theory. Recently, such involutions were used to obtain a constructive quantum Shannon decomposition with an application to quantum circuits. We will discuss some practical aspects of the use of this decomposition to obtain circuits for arbitrary unitary matrices. We discuss further applications of these techniques to the computation of mixed state entanglement and the parameterization of quantum operations on open systems.

3:42PM D17.00005 Quantum Foundations of Quantum Information¹, ROBERT GRIFFITHS, Carnegie-Mellon University — The main foundational issue for quantum information is: What is quantum information about? What does it refer to? Classical information typically refers to physical properties, and since classical is a subset of quantum information (assuming the world is quantum mechanical), quantum information should—and, it will be argued, does—refer to quantum physical properties represented by projectors on appropriate subspaces of a quantum Hilbert space. All sorts of microscopic and macroscopic properties, not just measurement outcomes, can be represented in this way, and are thus a proper subject of quantum information. The Stern-Gerlach experiment illustrates this. When properties are compatible, which is to say their projectors commute, Shannon’s classical information theory based on statistical correlations extends without difficulty or change to the quantum case. When projectors do not commute, giving rise to characteristic quantum effects, a foundation for the subject can still be constructed by replacing the “measurement and wave-function collapse” found in textbooks—an efficient calculational tool, but one giving rise to numerous conceptual difficulties—with a fully consistent and paradox free stochastic formulation of standard quantum mechanics. This formulation is particularly helpful in that it contains no nonlocal superluminal influences; the reason the latter carry no information is that they do not exist.

¹Support from NSF Grant PHY0757251 and Carnegie-Mellon University.

4:18PM D17.00006 Measuring the distance between unitary propagators of quantum systems of differing dimensions, MATTHEW GRACE, Thermal/Fluids Science & Engineering Department, Sandia National Laboratories, JASON DOMINY, Program in Applied & Computational Mathematics, Princeton University, ROBERT KOSUT, SC Solutions, Inc., CONSTANTIN BRIF, HERSCHEL RABITZ, Department of Chemistry, Princeton University — In this work, we develop a general distance measure that evaluates the distance between unitary quantum operations of differing dimensions which is (i) independent of the initial state of the system, (ii) straightforward to numerically calculate, and, most importantly, (iii) designed to directly evaluate quantum operations resulting from open-system dynamics. This measure is a natural extension of distance and corresponding fidelity measures employed in previous works that construct closed-system unitary operations. The properties of this measure are desirable for the calculation of distance, e.g., optimal control applied to open systems for quantum information processing, and enable a consistent comparison of quantum operations resulting from both closed- and open-system dynamics. As a numerical example, this distance measure is used to evaluate the fidelity of quantum operations resulting from the optimal control of one- and two-qubit unitary operations in the presence of a decohering environment. This example illustrates the utility of this measure for use in designing unitary quantum operations from open-system dynamics.


4:42PM D17.00008 Closed timelike curves enable perfect state distinguishability, TODD A. BRUN, University of Southern California, JIM HARRINGTON, Los Alamos National Laboratory, MARK M. WILDE, SAIC — The causal self-consistency condition for closed timelike curves can give rise to nonlinear interactions on chronology-respecting qubits. We demonstrate that particular unitary interactions between closed timelike curve qubits and chronology-respecting qubits allow perfect distinguishability of nonorthogonal states, and provide a constructive proof for an arbitrary number of nonorthogonal states. This has a number of highly significant consequences. For example, an adversary with access to closed timelike curves can break the B92, BB84, and SARG04 quantum key distribution protocols, or any prepare-and-measure quantum key distribution scheme. Our result also implies that a party with access to closed timelike curves can violate the Holevo bound by accessing more than \( \log(N) \) bits of information from an \( N \)-dimensional quantum state. In principle, he can transmit an arbitrarily large amount of classical information with a quantum system of fixed size. We discuss the implications of this for quantum cloning.
4:54PM D17.00009 Experimental Basis for IED Particle Model. J. ZHENG-JOHANSSON — The internally
electrodynamic (IED) particle model is built on three experimental facts: a) electric charges present in all matter particles, b) an accelerated charge generates
electromagnetic (EM) waves by Maxwell’s equations and Planck energy equation, and c) source motion gives Doppler effect. A set of well-known basic particle
equations have been predicted based on first-principles solutions for IED particle (e.g. J Phys CS128, 012019, 2008); the equations are long experimentally
validated. A critical review of the key experiments suggests that the IED process underlies these equations not just sufficiently but also necessarily. E.g.: 1) A
free IED electron solution is a plane wave \( \psi = Ce^{i(k_x \cdot \mathbf{r} - \omega t)} \) requisite for producing the diffraction fringe in a Davison-Germer experiment, and of also all basic
point-like attributes facilitated by a linear momentum \( \mathbf{k} \) and the model structure. It needs not further be a wave packet which produces not a diffraction
fringe. 2) The radial partial EM waves, hence the total \( \psi \) of an IED electron will, on both EM theory and experiment basis -not by assumption, enter two slits
at the same time, as is requisite for an electron to interfere with itself as shown in double slit experiments. 3) On annihilation, an electron converts (from mass
\( m \)) to a radiation energy \( h \omega \) without an acceleration which is externally observable and yet requisite by EM theory. So a charge oscillation of frequency \( \omega \) and its
EM waves must regularly present internal of a normal electron, whence the IED model.

5:06PM D17.0010 ABSTRACT WITHDRAWN —

5:18PM D17.0011 Quantum entanglement and informational activities of biomolecules, HANAN
entanglement and reveals its biological implications. The suggested holographic mechanism handles 2D slices of the physical world as a whole. Fitting this
simple holistic process in the Procrustean bed of individual particles interactions leads to intricacies of quantum theory with an unintelligible protrusion of distant
correlations. Holographic medium imposes dependence of quantum effects on absolute positioning. Testing this prediction for a non-exponential radioactive
decay could resolutely point to outside “memory.” The essence of Life is in the sophistication of macromolecules. Distinctions in biological information processing
of nucleotides in DNA and amino acids in proteins are related to entropies of their structures. Randomness of genetic configurations as exposed by their maximal
entropy is characteristic of passive identification rather than active storage functionality. Structural redundancy of proteins shows their operability, of which
different foldings of prions is most indicative. Folding of one prion can reshape another prion without a direct contact appearing like “quantum entanglement,”

Monday, March 16, 2009 2:30PM - 4:42PM –
Session D18 DPOLY: Focus Session: Transport and Optical Properties of Conjugated Polymers
and other Solution Processable Semiconductors 319

2:30PM D18.00001 Microstructure and Charge Transport in pBTTT Thin Film Transistors.
CHENCHEN WANG, Department of Applied Physics, Stanford University, ALBERTO SALLEO, LUDWIG GORIS, Department of Materials Science and
Engineering, Stanford University, IAIN MCCULLOCH, Chemistry Department, Imperial College, London, UK, MARTIN HEENEY, Materials Science Department,
Queen Mary University, London, UK, ALEXANDER ZIEGLER, Max Planck Institute, Martinsried, Germany — The present work focused on the morphology
and charge carrier mobility of poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophenes) (pBTTT) films. In annealed pBTTT films on oxide functionalized with
octyltrichlorosilane (OTS), TEM study shows that the large-scale terraces observed by AFM, which was believed to be the reason for high charge carrier mobility,
are composed of smaller crystalline grains. Using the mobility edge model, we find that, compared with the film on oxide, the density of trap states at the band
edge is reduced in the film on OTS, and it is about the same as the trap density in poly(3-hexylthiophene) (P3HT), which has lower carrier mobility. This result
are composed of smaller crystalline grains. Using the mobility edge model, we find that, compared with the film on oxide, the density of trap states at the band
edge is reduced in the film on OTS, and it is about the same as the trap density in poly(3-hexylthiophene) (P3HT), which has lower carrier mobility. This result

2:42PM D18.00002 Interfacial Charge Transfer in Nanoscale Polymer Transistors. JEFFREY WORNE,
RAJIV GIRIDHARAGOPAL, KEVIN KELLY, DOUGLAS NATÉLSON, Rice University, JOHN ANTHONY, University of Kentucky — Interfacial charge transfer
plays an essential role in establishing the relative alignment of the metal Fermi level and the energy bands of organic semiconductors. While the details remain
evasive in many systems, this charge transfer has been inferred in a number of photoemission experiments. We present electronic transport measurements in very
short channel (L < 100 nm) transistors made from poly(3-hexylthiophene) (P3HT). As channel length is reduced, the evolution of the contact resistance and the
zero gate voltage conductance are consistent with such charge transfer. Short channel conduction devices with Pt contacts is greatly enhanced compared to
analogous devices with Au contacts, consistent with charge transfer expectations. Alternating current scanning tunneling microscopy (ACSTM) provides further
evidence that holes are transferred from Pt into P3HT, while much less charge transfer takes place at the Au/P3HT interface. We have also begun to use these
same techniques to investigate the nature of interfacial charge transfer between metal electrodes and pentacene. We use these data together with our previous
results to develop a more complete picture of metal/organic interfaces.

2:54PM D18.00003 Ab initio study of molecular packing of organic semiconducting materials.
SEFA DAG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The self-organizing and electronic properties of organic semiconducting material,
poly(3-hexylthiophene) (P3HT), have been investigated in terms of their inter-monomer interaction and packing arrangements. We found that thiophene-thiophene interaction in
adjacent layers has a strong influence to create stacked planar structures. Our calculations showed that P3HT chains tend to stack into planar structures, in
which adjacent thiophene-thiophene rings along the stacking direction are 180° rotated with respect to each other. Theoretical powder diffraction profile of this
structure showed same structure with experimental reflection peaks. We also showed enhanced transport resulting from the organization of P3HT chains.

3:06PM D18.00004 Electrical Noise in Individual Conducting Polymer Nanowires. ALEXEY KO-
VALEV, YANYAN CAO, THERESA MAYER, THOMAS MALLOW, Penn State University — Electrical property characterizations of conducting polymer
nanowires have been limited primarily to resistance measurements. Electrical noise is one aspect that is usually overlooked, yet critical to their device
performance. Moreover, electrical noise is more sensitive to the polymer doping and microstructure than resistance, which makes it particularly interesting
for sensor applications. In this talk, we will present the results on the electrical noise measurements of individual multisegmented electrodeposited nanowires
based on Poly(3,4-ethylenedioxythiophene) (PEDOT) [1]. The polymer was electrochemically doped with either poly(4-styrenesulfonic acid) (PSS) or perchlorate
(CIO4). The nanowires had gold contacts on both ends and were measured in four-point and two-point configurations. We found that the electrical noise
behavior is typical of 1/f noise, with a spectral density that depends on the polymer structure and is affected by the ambient conditions. Our data show that
the contact noise represents a significant contribution to the total noise level. We will discuss the interpretation of these results assuming that the polymer is a
3:18PM D18.00005 Thin film morphology of electronic materials
S. D. HUDSON, R. J. KLINE, D. M. DELONGCHAMP, O. D. JURCHESCU, D. J. GUNDLACH, L. J. RICHTER, NIST, Gaithersburg, MD 20899 — The crystal orientation and morphology of a polythiophene (pBTTT) and an anthradithiophene (dif-TEADT, a pentacene analog) in thin films have been explored by TEM, SEM, AFM, GISAXD, NEXAFS, polarized FTIR and ellipsometry. The orientation has a striking influence on the performance of thin film transistors. We show that solution casting and annealing conditions have a significant effect on the morphology of pBTTT. Correlations between film surface step morphology and crystal orientation are determined. Interfacial interactions with the substrate (gold, silica, or fluorinated sam) govern the crystal orientation and crystal aggregate morphology of dif-TEADT. Depending on this orientation, the carrier mobility spans from approximately 0.001 cm²/Vs to 0.4 cm²/Vs. Epitaxial relationships within crystal aggregates are observed.

3:30PM D18.00006 Conjugated polymer/layered inorganic nanocomposites: solution processable route to enhanced thermoelectric performance
KEVIN SEE, JEFFREY URBAN, The Molecular Foundry, Lawrence Berkeley National Lab, RACHEL SEGALMAN, Department of Chemical Engineering, University of California, Berkeley — In recent years, incorporation of nanostructures has led to notable improvements in the performance of thermoelectric materials. At a given temperature T, the thermoelectric figure of merit ZT is given by $S^2T/\sigma\kappa$, where S is the Seebeck coefficient, $\sigma$ the electrical conductivity and $\kappa$ the thermal conductivity. In most cases, improvement in ZT through nanostructuring has been realized via reduction in thermal conductivity $\kappa$, rather than increases in the power factor $S^2\sigma$. Here we utilize solution-based intercalation chemistry to create layered inorganic/conjugated polymer nanocomposites with designed nanoscale interfaces engineered to enhance the power factor by energy filtering. The layered inorganic material Sb$_2$Te$_3$ was intercalated with poly(3-hexylthiophene), and the resulting composite material was cast into thin films from solution. The resulting devices exhibit Seebeck coefficients with two-fold enhancement over those reported for bulk Sb$_2$Te$_3$ with known conductivities for solution-processed films. These results demonstrate the promise of these novel intercalated materials for high performance solution processable thermoelectric materials.

3:42PM D18.00007 Revealing Transmission in Metal-Molecule Junctions Using Length Dependent Thermopower Measurements
JONATHAN A. MALEN, PETER DOAK, KANHYALAL BAHETI, T. DON TILLEY, ARUN MAJUMDAR, UC Berkeley — Conductance in metal-molecule junctions is known to trend with molecular endgroups, backbone, and length, but a more complete picture of the junction’s transmission structure has been hitherto elusive. We now report complimentary trends in the junction’s thermopower (S) that reveal length dependent changes in the molecular orbital alignment and coupling with contact states. Phenylene-diamines, phenylene-dithiols, and alkanedithiols trapped between gold contacts were examined. S increases linearly with length for phenylene-diamines and dithiols while it decreases linearly in alkanedithiols. In contrast, the data suggests that the molecular backbone determines the length dependence of S, while the endgroup determines the zero-length, or contact S. Transport in phenylenes was dominated by the HOMO, which moves closer to the Fermi energy of the contacts as $\sim 1/L$, and broadens due to contact coupling as $\sim 1/L^2$. In contrast, the decreasing trend in S for alkanedithiols suggests that transmission is largely effected by gold-thiol gap states between the HOMO and LUMO.

3:54PM D18.00008 Thermally-Induced Mesophase Transitions in Alkyl-Substituted Thienoacenes
CHARLES M. SHAW, XINNAN ZHANG, National Starch, LIDARIS SAN MIGUEL RIVERA, Dow Chemical, GEETHA G. NAIR, Centre for Liquid Crystal Research, Bangalore, India, ANANTAL JAKLI, Kent State University, ADAM J. MATZGER, DAVID C. MARTIN, University of Michigan — Pentathienoacene (T$_x$) is an organic molecule—first synthesized in recent years—that is most succinctly described as the thiphene analog of pentacene. In this study, the solid-state structure and phase behavior of diocetyl- and didodecyl-substituted T$_x$ were examined via differential scanning calorimetry (DSC), variable-temperature, polarized optical microscopy (VT-POM), variable-temperature X-ray diffraction (VT-XRD) and electron diffraction (ED). DSC reveals the presence of a number of phase transitions, while ED, VT-OM and VT-XRD reveal the details of the structural changes of these transitions. The first phase transition exhibited by both materials is a crystal-crystal transformation that involves the contraction of the unit cell along the long axis by nearly 25%. This change has been attributed to the introduction of numerous gauche defects at elevated temperatures. Further heating causes both molecules to exhibit a Smectic C liquid crystalline phase, identified by VT-OM and VT-XRD. VT-XRD was also utilized to elucidate lattice parameters for these various phases.

4:06PM D18.00009 Fullerene-based anchoring groups for molecular electronics
CHRISTIAN MARTIN, DAPENG DING, Leiden University and Delft University of Technology, The Netherlands, JAKOB SORENSEN, THOMAS BJORNHOLM, University of Copenhagen, Denmark, JAN VAN RUITENBEEK, Leiden University, The Netherlands, HERVE VAN DER ZANT, Delft University of Technology, The Netherlands — We present a route to a new fullerene-based anchoring group for molecular electronics. Using lithographic mechanically controllable break junctions in vacuum and at RT we have studied the electrical properties of 1,4-bis(fullero[6]pyrrolidin-1-yl)benzene. The compound can be self-assembled from solution and forms molecular junctions with a low-bias conductance of $G_0$. Compared to 1,4-benzenedithiol it exhibits a considerably lower conductance spread. Statistical analyses of the breaking process confirm the stability of the fullerene-gold bond.

4:18PM D18.00010 An organic nanoparticles transistor behaving as a spiking synapse
DOMINIQUE VUILAUME, FABIEN ALIBART, IEMN-CNRs, CHRISTOPHE NOVEMBRE, CEA-LIST, DAVID GUERIN, CNRS-IEMN, STEPHANE PLEUTIN, KAMAL M enjoymenti ,RI, IEMN-CNRs, CHRISTIAN GAMRAT, CEA-LIST, IEMN-CNRs TEAM, CEA-LIST TEAM — We demonstrate that an organic transistor, made of metal nanoparticles (NP) embedded into an organic semiconductor channel, behaves as a spiking synapse. We demonstrate that this device exhibits the main behavior of a biological synapse. For instance, it can be programmed to work as an excitatory or inhibitory synapse; it exhibits shot-term plasticity as well as spike timing dependent plasticity. This behavior is obtained by virtue of the combination of two properties: the transconductance gain of the transistor and the memory effect due to charges stored in the NP. The gold NP are immobilized into the source-drain channel by using surface chemistry (self-assembled monolayers) and they were subsequently covered by a thin film of pentacene. In a biological synapse, the excitatory behavior means that an incoming signal with a given frequency and duty cycle induces a post-synaptic signal having an increasing trend, whereas in the case of an inhibitory synapse, the post-synaptic signal tends to decrease. This behavior is exactly what we demonstrated for the ONT.

4:30PM D18.00011 The role of the oxygen/water redox couple in suppressing electron conduction in field-effect transistors
PIERRE L. LEVESQUE, Université de Montréal, CARLA M. AGUIRRE, École Polytechnique de Montréal, MATTHIEU PAILLET, FRANÇOIS LAPOINTE, Université de Montréal, BENOIT C. ST-ANTOINE, PATRICK DESJARDINS, École Polytechnique de Montréal, RICHARD MARTEL, Université de Montréal — Much like with organic semiconductor FETs, a characteristic of carbon nanotube based devices has been their almost exclusive p-type character in air. Electron transport can be observed only under certain conditions, for instance devices annealed in vacuum. We investigated the impact of the chemical nature of the substrate and of ambient adsorbates on the field-effect switching behavior of both nanoscale and thin-film FETs. Our study, using carbon nanotubes as the testbed, revealed that the intrinsic material properties are modified when an adsorbed water layer containing solvated oxygen is present on the SiO$_2$ surface and lead to the reduction of n-type conduction. This finding demonstrates that an electrochemical charge transfer reaction between the semiconducting channel and the aqueous oxygen redox couple is the underlying phenomenon governing the suppression of electron conduction in these devices. This effect should be considered when measuring the transport properties of nanostructures such as nanowires, organic materials, nanotubes, graphene conducted on SiO$_2$/Si substrates.
Monday, March 16, 2009 2:30PM - 5:30PM —
Session D19 DPOLY: Focus Session: Grazing Incidence Scattering and New Imaging Techniques 320

2:30PM D19.00001 Probing kinetics and dynamics of nanocomposites with grazing-incidence small-angle x-ray scattering.1 JIN WANG, Argonne National Laboratory — Synthesizing complex nanocomposites and superstructures is of great interest in all areas of materials science and technology. Since the entire synthesis and assembly process can take place far from equilibrium conditions, a controlled process has to be guided by a thorough understanding of the kinetics and dynamics in the composites. This requires measurement of the structure in situ and in real time with subnanometer spatial resolution and millisecond to subsecond temporal resolution. As an increasingly important structural-characterization technique, grazing-incidence small-angle x-ray scattering (GISAXS) finds vast applications in the research of nanostuctures and nanocomposites at surfaces and interfaces. Most significantly, as a complementary method to conventional surface-sensitive tools such as scanning probe microscopy and electron microscopy, GISAXS can be used in situ and in real time to monitor the formation of the nanostructure or nanocomposite, which makes it most suitable for studying the kinetics of nanoassembly processes. The GISAXS technique can also be an integral part of numerous research, for example, those involving kinetics of mesoscaled ordered block copolymer thin films, kinetics of sol-gel processes, quantum dots, nanoparticles in ultrathin films, and dynamics and phase transitions 2D nanocrystal superlattices. Here, I will focus on the applications of GISAXS in real-time structure characterization, the dynamics in polymer/nanoparticle nanocomposites, and the challenges to elucidate nanostructure formation in nanoscience and nanotechnology.

3:06PM D19.00002 Single beam approach for GISAXS1 BYEONGDU LEE, CHIEH-TSUNG LO, Argonne National Laboratory, PAPPANNA THIYAGARAJA, ZHONGWEI NUI, QIAN WANG, University of South Carolina — The multiple scattering effects present in the grazing incidence small-angle x-ray scattering (GISAXS) data and dynamics addressed theoretically as well as experimentally with measurement of a series of patterns at different incident angles, referred to as “incident-angle-resolved GISAXS” (IAR-GISAXS). We found that under certain conditions, it is possible to extract the correct structural features of the materials from the GISAXS data using the kinematic SAXS formalisms assuming a single beam, without the need to use the distorted wave Born approximation (DWBA) to account for the scattering by the reflected beam. Furthermore, the Kiessig fringes in GISAXS enable the measurement of average distance between the particle and the substrate, similar to the measurement of film thickness using the fringes in the x-ray reflectivity data. We believe that the methods developed here will expand the application of GISAXS as they enable the use of model-dependent and independent SAXS theories to nanostructured 2D-ordered films.

3:18PM D19.00003 Surface Dynamics of Free PS Chains on Chemically Identical Polymer Brushes: An XPCS Study. GOKCE UGUR, Department of Polymer Science, The University of Akron, Akron, OH 44325-3909, BULENT AKGUN, Center for Neutron Research, National Institutes of Standards and Technology, Gaithersburg, Maryland 20899, ZHANG JIANG, SURESH NARAYANAN, Experimental Facilities Division, Argonne National Laboratory, Argonne, IL 60439, WILLIAM J. BRITTAIN, MARK D. FOSTER, Department of Polymer Science, The University of Akron, Akron, OH 44325-3909 — We found no relaxation of fluctuations of the brush surfaces within the range of time (0.2-1100 s) and length scale (0.6-3 um) studied by X-ray photon correlation spectroscopy (XPCS). This is true for PS brushes of thicknesses of 9-101 nm and grafting density of 0.12-0.6 chains/nm² at temperatures up to 130°C above bulk Tg = 60°C. Results on the dynamics of a layer of untethered 2.2k PS chains on top of a PS brush surface show that placing the PS chains atop the brush dramatically slows down the surface relaxations of the film surface. As the ratio of the thickness of the layer of untethered chains to the thickness of the highly dense brush drops below ~0.5, the surface relaxations become too slow to be observed readily with XPCS. Reducing grafting density of the underlying brush markedly slows the surface dynamics. The surface dynamics of the layer of free PS chains are coupled with those of the underlying brush. 3:30PM D19.00004 X-ray Standing Wave Studies of Stability and Dynamics in Poly(4-bromostyrene)/Poly(4-vinylpyridine) Thin Films YAN SUN, KENNETH SHULL, Northwestern University, JIN WANG, Argonne National Laboratory — The thermodynamic stability and wetting behavior in systems consisting of two or three distinct layers of polymeric thin films have been investigated with atomic force microscopy (AFM) and x-ray standing waves (XSW) generated via total external reflection from an x-ray mirror. We have probed the structural evolution of thin poly(4-bromostyrene) (P(BrS)) films with various degrees of bromination, prepared on top of a poly(4-vinylpyridine) (P4VP) layer whose dynamics is influenced by its interaction with the underlying substrate and couple to that of PBrs. The addition of a top poly(styrene) (PS) layer was also used in some cases. The samples were subjected to annealing treatments above the polymer glass transition temperatures. Reflectivity and x-ray fluorescence from bromine markers in the PBrs layer were tracked. Dewetting of the PS occurred with sufficient annealing time, though the results suggest that this proceeded faster with low PBrs bromination. AFM studies on the PBrS/P4VP system revealed a clear PBrS thickness dependence on the dewetting morphology and dynamics of this layer.

3:42PM D19.00005 Quantitative electron tomography and its application to polymer nanostructures. HIROSHI JINNAI, Department of Macromolecular Science and Engineering, Kyoto Institute of Technology — The transmission electron microscopy (TEM) is a powerful tool to visualize three-dimensional (3D) structures in many fields of materials science. Recently, researchers are trying not only to visualize 3D nanostructures but also to quantify them in order to seek a possible correlation between the 3D structures and materials' properties. However, one of the serious problems that prohibit TEM imaging of 3D images is the “missing wedge” in the Fourier space that is caused by the limitation of angular range available in transmission electron microscopes (TEM). Please note that the computerized tomography (CT), on which TEMT is based, requires projections from entire tilt angles, i.e., ±90°. Thus, the most faithful tactics for the CT is to tilt specimen over ±90°. In order to realize such requirement, a rod-shaped ZrO2/polymer nano-composite whose diameter is ca. 150 nm was attached at the tip of a specially modified specimen holder without any supporting film. A complete set of tomograms has been generated for the first time from the 181 projections that were taken over the angular range of ±90°. One of the structural parameters characterizing the nanocomposite, a volume fraction of ZrO2, ϕ, was measured as a function of the maximum tilt angle, α. It was found that ϕ was in excellent agreement with the known volume fraction of ZrO2 when α=90°, i.e., ±90° tilt, while ϕ increased with decreasing α. When α=60°, that is a typical maximum tilt angle, the measured ϕ was larger by 20~30% than the true value. In addition to the above TEMT experimental technique, some applications of TEMT to polymer nano-structures will be presented at the conference time.
4:18PM D19.00006 Three-dimensional subwavelength imaging with phase-less power extinction tomography, ALEXANDER A. GOVYADINOV, GEORGE Y. PANASYUK, JOHN C. SCHOTLAND, University of Pennsylvania — Modern near-field methods extend the spatial resolution of optical microscopes beyond the classical diffraction limit. However, the majority of these methods only recover two-dimensional maps of optical intensity near the sample surface. The interpretation of these maps for manifestly inhomogeneous samples has been proven to be problematic. Here we derive an analytical technique which allows unique subwavelength 3D reconstruction of both real and imaginary parts of susceptibility.

4:30PM D19.00007 Helium ion microscopy and its application to organic materials, STEVEN HUDSON, ANDRAS VLADAR, BIN MING, NIST, Gaithersburg, MD 20899 — Helium ion microscopy (Helm) is a new scanning probe microscopy that uses a He+ beam. This microscope has improved resolution and depth of field in comparison to SEM, as demonstrated through imaging of metal particles. Organic materials, including patterned polyelectrolyte multilayers and organic semiconductor crystals, have also been imaged. The surface sensitivity, image contrast and qualitative secondary electron yield have been evaluated, in an effort to understand beam/specimen interactions and compare them with electron beam/sample interactions.

4:42PM D19.00008 Robust Tips for High Resolution Chemical Imaging1, CARLOS BARRIOS, ANDREY MALKOVSKIY, ALEXANDER KISLIUK, ALEXEI SOKOLOV, MARK FOSTER, Department of Polymer Science, The University of Akron — Tip enhanced Raman spectroscopy (TERS) combines scanning probe microscopy with Raman spectroscopy, taking advantage of apertures on near-field optics. A plasmonic structure at the apex of a sharp tip provides signal amplification required for chemical imaging. Plasmonic structure characteristics such as roughness, shape, and radius determine the spatial resolution and signal enhancement. Unfortunately, noble metal nanostructures have limited lifetimes due to mechanical, chemical, and thermal degradation. Lifetime extension requires slowing degradation processes while minimizing unfavorable influences on the optical response. An ultrathin SiO2 protective coating provides lifetime improvement of silver plasmonic nanostructures on SPM tips. Controlled physical vapor deposition (PVD) of Al can be used to create ultrathin (~2-3 nm) Al2O3 coatings that improve significantly the stability and wear resistance of plasmonics structures without substantial degradation of optical properties. Such a coating completely prevented decay in plasmonic activity after 40 days of use.

5:06PM D19.00010 Intensity Fluctuations of Optical Microscopy as a Means to Measure Axial Diffusion, MALVIKA BIHARI, PSE, UMASS Amherst, THOMAS RUSSELL, PSE, UMASS Amherst, DAVID HOAGLAND, PSE UMASS Amherst — Via optical microscopy, geometrically hindered motions of a single large solute (particle or polymer) can be imaged in real time. Here, intensity fluctuations of confocal microscopy admit another way to probe such motions, one convenient when motions are perpendicular to a planar substrate. The focal plane is positioned within the substrate (lying on the microscope stage) and intensity fluctuations arise from motions in-and out-of the focal volume. Two experiments illustrate the new approach, diffusion within pores of a planar membrane or in solution near a solid wall. In the first, diffusion coefficients of spherical particles were measured inside pores of a track-etched polycarbonate membrane as functions of particle and pore size. In the second, anisotropic diffusion (perpendicular/parallel) of the same particles was measured within a few particle diameters of a solid boundary. Theory for hydrodynamically hindered diffusion in both cases is well developed, and data are compared to predictions. Two ways to assess particle/polymer motion, tracking single particles and correlating intensity fluctuations, will be discussed.

5:18PM D19.00111 Three-Dimensional Imaging of Polymeric Nanostructures by Molecular Switching in Far Field Fluorescence Microscopy, CHAITANYA ULLAL, ROMAN SCHMIDT, ALEXANDER EGNER, BENJAMIN HARKE, JAN KELLER, Max Planck Institute for Biophysical Chemistry — Morphological studies of self-assembled polymeric structures with length scales of interest below 100 nm have typically been conducted either by scattering-based techniques or electron and scanning probe microscopes. These techniques, however, do not provide easy access to truly 3D-informational content. In contrast, Far-field optical methods retain the advantage of simultaneously providing local, dynamic, and in situ three-dimensional (3D) structural information. The diffraction limited optical resolution of its standard variants, however, restricts the minimum feature size that can be examined. We exploit molecular transitions of the fluorophores to circumvent the diffraction barrier and demonstrate the power of emerging far-field fluorescence microscopy with nanoscale resolution for the study of self-assembly. We simultaneously improve both the lateral (x,y) and the axial (z) resolution of stimulated emission depletion (STED) microscopy. The increased 3D resolution is used to unambiguously map the morphology of self-assembled polymeric nanostructures in a facile manner.


2:30PM D20.00001 Simulation study of proton transport in stretched nanocomposite ionomer fuel-cell membranes1, PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — We have used coarse-grained simulation methods to investigate the effect of inclusions of nanoparticles on the stretching-induced structure orientation and on the proton conductivity of polymer electrolyte membranes. Uniaxial stretching of a Nafion film containing no inclusions causes a modest increase in proton conductivity in the direction of stretching. This effect does not persist to any significant degree after removal of the stretching stress. Stretching of a Nafion film containing spherical nanoparticle inclusions, on the other hand, causes a large increase in proton conductivity in the direction of stretching, and this effect persists to a much greater extent after the removal of the stretching stress. Simulations were performed with monodisperse nanoparticle whose diameters were in the range from 17 to 28 nm, and whose surfaces were either hydrophilic, neutral, or hydrophobic. The greatest effect in causing enhancement of the proton conductivity and in causing persistent ordering was found for hydrophilic nanoparticle inclusions of 28 nm diameter.

1Work supported by DOE Grant DE-FG02-05ER46244

4:42PM D19.00008 Robust Tips for High Resolution Chemical Imaging1, CARLOS BARRIOS, ANDREY MALKOVSKIY, ALEXANDER KISLIUK, ALEXEI SOKOLOV, MARK FOSTER, Department of Polymer Science, The University of Akron — Tip enhanced Raman spectroscopy (TERS) combines scanning probe microscopy with Raman spectroscopy, taking advantage of apertures on near-field optics. A plasmonic structure at the apex of a sharp tip provides signal amplification required for chemical imaging. Plasmonic structure characteristics such as roughness, shape, and radius determine the spatial resolution and signal enhancement. Unfortunately, noble metal nanostructures have limited lifetimes due to mechanical, chemical, and thermal degradation. Lifetime extension requires slowing degradation processes while minimizing unfavorable influences on the optical response. An ultrathin SiO2 protective coating provides lifetime improvement of silver plasmonic nanostructures on SPM tips. Controlled physical vapor deposition (PVD) of Al can be used to create ultrathin (~2-3 nm) Al2O3 coatings that improve significantly the stability and wear resistance of plasmonics structures without substantial degradation of optical properties. Such a coating completely prevented decay in plasmonic activity after 40 days of use.

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5:18PM D19.00111 Three-Dimensional Imaging of Polymeric Nanostructures by Molecular Switching in Far Field Fluorescence Microscopy, CHAITANYA ULLAL, ROMAN SCHMIDT, ALEXANDER EGNER, BENJAMIN HARKE, JAN KELLER, Max Planck Institute for Biophysical Chemistry — Morphological studies of self-assembled polymeric structures with length scales of interest below 100 nm have typically been conducted either by scattering-based techniques or electron and scanning probe microscopes. These techniques, however, do not provide easy access to truly 3D-informational content. In contrast, Far-field optical methods retain the advantage of simultaneously providing local, dynamic, and in situ three-dimensional (3D) structural information. The diffraction limited optical resolution of its standard variants, however, restricts the minimum feature size that can be examined. We exploit molecular transitions of the fluorophores to circumvent the diffraction barrier and demonstrate the power of emerging far-field fluorescence microscopy with nanoscale resolution for the study of self-assembly. We simultaneously improve both the lateral (x,y) and the axial (z) resolution of stimulated emission depletion (STED) microscopy. The increased 3D resolution is used to unambiguously map the morphology of self-assembled polymeric nanostructures in a facile manner.


2:30PM D20.00001 Simulation study of proton transport in stretched nanocomposite ionomer fuel-cell membranes1, PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — We have used coarse-grained simulation methods to investigate the effect of inclusions of nanoparticles on the stretching-induced structure orientation and on the proton conductivity of polymer electrolyte membranes. Uniaxial stretching of a Nafion film containing no inclusions causes a modest increase in proton conductivity in the direction of stretching. This effect does not persist to any significant degree after removal of the stretching stress. Stretching of a Nafion film containing spherical nanoparticle inclusions, on the other hand, causes a large increase in proton conductivity in the direction of stretching, and this effect persists to a much greater extent after the removal of the stretching stress. Simulations were performed with monodisperse nanoparticle whose diameters were in the range from 17 to 28 nm, and whose surfaces were either hydrophilic, neutral, or hydrophobic. The greatest effect in causing enhancement of the proton conductivity and in causing persistent ordering was found for hydrophilic nanoparticle inclusions of 28 nm diameter.

1Work supported by DOE Grant DE-FG02-05ER46244
2:42PM D20.00002 The role of nanoparticle-membrane coupling in nanocomposite ionomers1, ELSHAD ALLAHYAROV, PHILIP TAYLOR, Case Western Reserve University — Coarse-grained simulation methods have been used to investigate the effect of inclusions of spherical nanoparticles on the properties of Nafion®-like membranes. We find the clustering of the sulfonate head groups to be strongly affected by the presence of a monodisperse array of spheres when the sphere diameters lie in the range from 17 to 28 nm. This change in morphology enhances the proton conductivity of the membrane through the formation of channels connecting adjacent clusters. This effect was characterized in terms of the distribution of channel lengths of the hydrophilic phase. Simulations were performed for Nafion containing spherical nanoparticles whose surfaces were either hydrophilic, neutral (hard core), or hydrophobic. The diameters of the nanoparticles were changed while keeping fixed the volume fraction of inclusions. We find that the proton conductivity of these nanocomposites is always higher than the conductivity of ionomers without additives. This effect becomes most pronounced in nanocomposites containing particles whose surfaces are hydrophilic, and whose diameters are in the larger part of the range of sizes examined.

1Work supported by DOE Grant DE-FG02-05ER46244.

2:54PM D20.00003 Multi-Lamellar Structures in Nafion, JOSEPH A. DURA, NIST - Center for Neutron Research, VIVER S. MURTHI, UTC Power Corp., MICHAEL R. HARTMAN, University of Michigan, Nuclear Engineering and Radiological Sciences, SUSHIL K. SATIJA, CHARLES F. MAJKRZAK, NIST - Center for Neutron Research — Both proton conductivity and gas diffusion are key factors in the performance of a fuel cell and proton exchange membrane, PEM. They are critically dependent on water content and morphology, especially in the three phase region where catalyst, PEM, and gases such as fuel or oxidizer co-exist. Here we show that lamellar structures composed of thin alternating water rich and Nafion rich layers exist at the interface between SiO2 and the hydrated Nafion film. Lamellae thickness and number of layers increase with humidity. Some lamellae remained in the film after dehydration. Multilayer lamellae are not observed for Nafion on Au or Pt surfaces. Instead, a thin partially hydrated single interfacial layer occurs and decreases in thickness as a few angstroms as humidity is reduced to zero. The absorption isotherm of the rest of the Nafion film is similar to that of bulk Nafion for all three surfaces investigated.

3:06PM D20.00004 RT-TDDFT simulation of the optical properties of a model organic photovoltaic device, F. VILA, J.J. REHR, U. of Washington — Organic solar cells are attracting much interest because of their potential as cost-effective photovoltaic devices. Prototypical cells consist of a bilayer of p- and n-type materials. The conversion of light into a current is initiated by the absorption of a photon in the p-type donor, mediated by the creation, diffusion and dissociation of an exciton, and finalized by a charge transfer to the n-type acceptor, with subsequent transport to the electrodes. To explore this issue, we simulate the optical response of a model bilayer cell composed of a polythiophene(pT)/C60 donor/acceptor pair using an efficient implementation of real-time TDDFT. We find that the chain twist induced by the C60 on the pT shifts the absorption onset from 1.8 to 2.0 eV. This shift is larger and of opposite sign compared to that induced by the inclusion of either regioregular or random side-chains in pT, and by the interaction between two pT chains. Finally, we discuss extensions for the simulation of charge transport and exciton mobility.

3:18PM D20.00005 Collecting photo-generated charge carriers from metallo-organic materials, A.R. CARTER, J.H. PARK, Dept. of Physics, The Ohio State University, Columbus, Ohio 43210-1117, Y.-H. CHOU, Y. GHOSH, C.R. REED, L.M. MIER, T.L. GUSTAFSON, M.H. CHISOLM, Dept. of Chemistry, The Ohio State University, Columbus, Ohio 43210-1185, A.J. EPSTEIN, Dept. of Physics and Dept. of Chemistry, The Ohio State University, Columbus, Ohio 43210-1117 — Organic photovoltaic materials continue to garner attention as potential low cost and tunable alternatives to conventional inorganics. We report progress in utilizing hybrid metal-organic materials that incorporate metal-metal (M-M) quadruply bonded units into oligothiophenes via carboxylate linkers. Varying the metal (M = Mo, W) or the ligands shifts the energetics and can be exploited to extend absorption into the infrared. These materials have high absorptivity from 300 nm (4.1 eV) to 900 nm (1.4 eV). We present the results of photophysical studies of structures that employ these materials.

1Supported by DOE Grants DE-FG35-08GO18024 (FV and JIR), DE-FG02-97ER45623 (JIR).


3:30PM D20.00006 Monolithic Tandem Organic Photovoltaic Cell Utilizing Transparent Carbon Nanotube Interlayer, KAMIL MIELCZAREK, University of Texas at Dallas, Physics Department, Nanotech Institute, SENKU TANAKA, Shimane University, University for Integrated Research in Science, RAQUEL OVALLE ROBLES, ALEXANDER KUZNETSOV, University of Texas at Dallas, Nanotech Institute, BRIAN WANG, University of Texas, DEAN HSU, University of Texas at Dallas, RAY BAUGHMAN, ANVAR ZAKHIDOV, University of Texas at Dallas, Nanotech Institute, ALAN G. MCDIARMID NANOTECH INSTITUTE TEAM — We demonstrate an organic photovoltaic multijunction cell in a monolithic parallel tandem structure in which transparent multi and single-walled nanotube sheets are used as an interlayer electrode connecting two cells; polymeric photovoltaic (PPV) cell or organic low molecular PV (OPV). Each cell is characterized independently and the short circuit current density of the tandem is shown to be larger than individual cells for the PPV-MWCNT-OPC tandem*. Overall efficiency is increased attributed to effective use of transparent CNTs and enhanced spectral sensitivity due to differing active layer materials. Computer model circuit simulation is used to analyze the parameters of cells in parallel and series configurations. Advantages of a parallel connection is shown for PV cells with differing photocurrents. The PPV-CNT-PPV and OPV-CNT-OPV cells are also created and described. *S.Tanaka, K Mielczarek, et al., APL. (submitted 2008, October).

3:42PM D20.00007 Tandem of solid dye-sensitized solar cell with carbon nanotubes interlayer, CHAO-CHEN YUAN, JIANGBIN XIA, ANVAR ZAKHIDOV, Univ. of Texas at Dallas NanoTech Institute — The light-to-electron conversion efficiency of the dye-sensitized solar cell (DSC) was recently improved up to 11.1%. However, this efficiency is not sufficient for cost-effective commercial production, so the expansion of the absorption region of the solar cell is needed. For transparent carbon nanotubes, parallel-connected tandem DSCs is developed. Novel parallel type of tandem cell structure is created. We create a parallel combination for cells using different dyes. The top cell is transparent and the bottom cell only uses light passing through the top cell. Instead of a common platinum counter electrode as interlayer, we use transparent carbon nanotubes (CNTs) coated on hole transport layers of each sub-cell, as an interlayer counter electrode. With high enough conductivity and high optical transparency, the compatibility of CNTs work as the interlayer counter electrode performing even better than Pt. The short-circuit current density (Jsc) for the tandem cell is demonstrated to be higher than that of separate the front and back photo electrodes. A model using light energy absorbed by the photo electrode is N719 top cell and a black-dye bottom cell is developed. Now the prototype of DSC tandem cell has been proved with the efficiency of 0.293% with 0.2 cm2 area.

1The novel material as an interlayer for tandem cell - Carbon nanotubes
3:54PM D20.00008 NEXAFS Spectroscopy of Biomimetic Dyes for Solar Cells. PETER COOK, XIAOSONG LIU, FRANZ HIMPSEL, Physics Department, University of Wisconsin Madison — Organic photovoltaics hold the potential for an inexpensive alternative to traditional silicon in solar cell production. A group of such dyes is investigated systematically including porphyrins, phthalocyanines, and cytochrome c, all of them characterized by a transition metal atom surrounded by a cage of four nitrogen atoms. X-ray absorption spectroscopy of the transition metal 2p and the nitrogen 1s absorption edges reveals the LUMO, the oxidation state of the transition metal, and its spin state. In addition, the sensitivity of these molecules to damage by photon-induced hot electrons is investigated. While the nitrogen cage is rather robust, the peptide bonds between the one hundred amino acids in cytochrome c are easily damaged. This finding suggests minimizing the size of biologically-inspired molecules for photovoltaic applications.

4:06PM D20.00009 Semiconductor Conjugated Polymer-Quantum Dot Nanocomposites at the Air/Water Interface and Their Performance in Thin Film Solar Cells. ZHIQUN LIN, MATTHEW GOODMAN, JUN XU, JUN WANG, Iowa State University — Organic-inorganic nanocomposites consisting of electroactive conjugated polymer, poly(3-hexyl thiophene) (P3HT) intimately tethered on the surface of semiconductor CdSe quantum dot (i.e., P3HT-CdSe nanocomposites) at the air/water interface formed via Langmuir isotherms were explored for the first time. The P3HT-CdSe nanocomposites displayed a high pressure plateau in the Langmuir isotherm, illustrating their complex packing at the air/water interface. Furthermore, photovoltaic devices fabricated from the LB depositions of the P3HT-CdSe nanocomposites exhibited a relatively high short circuit current, 1Sc, while maintaining a thin film profile. These studies provide insights into the fundamental behaviors of semiconductor organic-inorganic nanocomposites confined at the air/water interface as well as in the active layer of an organic-based photovoltaic device.

4:18PM D20.00010 Effect of polymer mobility on conductivity of single-ion conductors. KOKONAD SINHA, JANNA MARANAS, The Pennsylvania State University — Scientists are turning to the use of polymers as substitutes for liquid electrolytes in lithium ion batteries, because of their mechanical flexibility and non-toxic properties. Physical mixtures of lithium salt and poly(ethylene oxide) (PEO + LiClO4) are commonly chosen because they have potential for high ionic conductivities. However, high mobility of ions in these mixtures results in electrode polarization, which affects battery performance. To isolate the effect of the cation and to reduce the obstacle of concentration polarization, the anion is chemically incorporated into the backbone of the polymer, thereby rendering it immobile. These single-ion conductors are called ionomers. Neutron scattering experiments have been conducted on ionomers to observe the relation between ionomer mobility and ionic conductivity. Results show that with increasing ion content, there arises a new process at smaller length scales. Comparisons with PEO + LiClO4 systems hint at the formation of cation-PEO-anion complexes which are significantly slower in dynamics than the segmental motion of the polymer. This interaction between the cation and the polymer chain is of vital importance in understanding the fundamental mechanism of ion conduction in polymers.

4:30PM D20.00011 Electrochemical Characterization of poly (styrene-b-ethylene oxide)/LiTFSI Lamellar Diblock Copolymer Electrolyte System. NITASH BALSARA, University of California, Berkeley, CA, ASHUTOUSH PANDAY, Lawrence Berkeley Lab, Berkeley, CA, SCOTT MULLIN, NISITA WANKULIE, University of California, Berkeley, CA — We present the electrochemical characterization studies of symmetric poly (styrene-b-ethylene oxide) copolymers (SEO) and Li[N(SO2CF3)2] (LiTFSI). The molar ratio of Li to ethylene monomers, r, was varied from 0.02 to 0.10. The ionic conductivity of these electrolytes increases with molecular weight over the entire range of temperatures and r values examined. Preliminary data suggest that the salt diffusion coefficient also increases with increasing MW of PEO block.

4:42PM D20.00012 Progress toward few-molecule photochemistry with a low temperature STM. DAVID DAUGHTON, DONGHUN LEE, JAY GUPTA, The Ohio State University — Photochemistry at interfaces provides insight into molecular binding and charge transfer with future implications for organic photo-active devices. We have developed a novel instrument combining a low-temperature scanning tunneling microscope (STM) with a maneuverable, high numeric aperture lens in proximity to the tunnel junction for the study of photoactive systems with single molecule sensitivity. We will present the results of our initial efforts on the electronic and photo-induced polymerization of C60 islands, tunneling and photo-induced isomerization of thiondigo, and the effects of well-defined optical nanostructures on photochemical processes. http://www.physics.ohio-state.edu/~jgupta

1Supported by the Beckman Foundation.

4:54PM D20.00013 Confinement-Induced Fast Discharge and Low Dielectric Losses in Ferroelectric PVDF Graft Copolymers. LEI ZHU, FANGXIAO GUAN, ZHONGZHE YUAN, Polym. Program, Inst. of Mater. Sci. and Dept. of Chem., Mater. and Biomolecular Eng., University of Connecticut, Storrs, CT 06269-3136 — The relatively high dielectric loss of poly(vinylidene fluoride) (PVDF) and its copolymers limits their range of application as a high energy density capacitor material, although a high electric energy density was recently reported for millisecond discharge. In this work, we report time independent (or fast) discharge and reduced losses in ferroelectric poly(vinylidene fluoride) (PVDF) graft copolymer dielectric films. Experimental results suggested that the fast discharge and low losses were results of an increased amorphous content and nanoscale confinement of ferroelectric PVDF crystals.

1This work is supported by ONR (N00014-05-1-0338).

5:06PM D20.00014 ABSTRACT WITHDRAWN —

Monday, March 16, 2009 2:30PM - 5:30PM — Session D21: Semiconductors: Transport 323

2:30PM D21.00001 Unified Theory of Charge Transport in Wide-Band and Narrow-Band Semiconductors. FRANK ORTMANN, FRIEDHELM BECHSTEDE, KARSTEN HANNEWALD, ETSF and IFTO, Friedrich- Schiller-University Jena, Germany — The charge carrier mobility is often calculated within one of the two limiting cases: wide bands or narrow bands. In the case of wide-band systems, usually pure band transport is assumed along with a calculated relaxation time. In contrast, for narrow-band materials, hopping is usually considered prevalent and the interaction with lattice vibrations is described within the polaron concept. In this talk, we will present a unified approach to the description of charge transport based upon the Kubo formalism applied to a Holstein Hamiltonian. As a result, we obtain an analytical formula for the temperature dependence and anisotropy of the mobility describing a seamless transition from band transport at low temperatures to hopping transport at high temperatures. The results are illustrated for naphthalene crystals and a comparison to previous approaches [1,2] is made.

2:42PM D21.00002 Carrier transport in nanodevices: a competitive playground for the Boltzmann and the Wigner distribution functions. FONS BROSENS, Universiteit Antwerpen, WIM MAGNUS, Interuniversity Microelectronics Centre (IMEC) — In principle, transport of charged carriers in nanometer sized solid-state devices can be fully characterized once the non-equilibrium distribution function describing the carrier ensemble is known. In this light, we have revisited the Boltzmann and the Wigner distribution functions and the framework in which they emerge from the classical respectively quantum mechanical Liouville equation. We have assessed the method of the characteristic curves as a potential workhorse to solve the time dependent Boltzmann equation for carriers propagating through spatially non-uniform systems, such as nanodevices. In order to validate the proposed solution strategy, we numerically solve the Boltzmann equation for a one-dimensional conductor mimicking the basic features of a biased low-dimensional transistor operating in the on-state. Finally, we propose a computational scheme capable of extending the benefits of the above-mentioned solution strategy when it comes to solve the Wigner-Liouville equation.

2:54PM D21.00003 Measurement and analysis of extraordinary electroconductance in Ti-GaAs hybrid structures1, J.S. SOLIN, A.K.M. NEWAZ, Y. WANG, J. WU, Washington University in St. Louis, W.-J. CHANG, V.R. KAVASSERI, I.S. AHMAD, I. ADESIDA, R. BASHIR, University of Illinois at Urbana-Champaign — We present a comprehensive study of a new phenomenon, extraordinary electroconductance (EEC), in microscopic and mesoscopic metal-semiconductor hybrid structures (MSS) at room temperature with different geometrical characteristics. Our artificially designed MSS structures show highly efficient external electric field sensing properties not exhibited by bare semiconductor structures. The EEC device has been fabricated from a GaAs epitaxial layer with a Ti/Au shunt. When subject to an external electric field it gives a maximum 5.2% EEC effect corresponding to an external electric field resolution of 3.05 V/cm at a bias field of 2.5 kV/cm. Moreover, the study reveals a strong dependence of the transport properties on the geometry of the MSS. An analytical 2-layer model is developed which provides good agreement with the experimentally observed data. We propose that scaled down nanoscopic EEC sensor arrays can be used as a novel technique for imaging the charge distribution on a single cell surface in real time.

3:06PM D21.00004 Universal oscillations in counting statistics, CHRISTIAN FLINDT, Harvard University, CHRISTIAN FRICKE, FRANK HOHLS, Leibniz University Hannover, Germany, TOMAS NOVOTNY, Charles University, Czech Republic, KAREL NETOCNY, Academy of Science, Czech Republic, TOBIAS BRANDES, Technical University Berlin, Germany, ROLF J. HAUG, Leibniz University Hannover, Germany — Noise and fluctuations are results of stochastic processes that originate from quantum or classical sources. Higher-order cumulants of the probability distribution underlying the stochastic events are believed to contain detailed information about the stochastic process, but they are often difficult to measure. In this talk we report the first measurements of the transient cumulants of the number of electrons passing through a quantum dot to very high orders (up to order 15) [1]. The cumulants grow factorially in magnitude with the cumulant order and show surprising oscillations as functions of measurement time. Based on theory for high-order derivatives in the complex plane we show that the oscillations in fact constitute a universal phenomenon, appearing as a function of almost any parameter for a large class of stochastic systems. Our analytical 2-layer model is developed which provides good agreement with the experimentally observed data [2]. We propose that scaled down nanoscopic EEC sensor arrays can be used as a novel technique for imaging the charge distribution on a single cell surface in real time.

3:18PM D21.00005 Bloch Oscillations of Electrons in a Quantum-Dot Superlattice1, DANHONG HUANG, Air Force Research Laboratory, S.K. LYO, Sandia National Laboratories — Numerical results for both the transient and steady-state currents in a strong DC electric field are presented for electrons in a quantum-dot superlattice. A microscopic scattering model is applied to study the dynamics of electrons scattered by impurities and phonons based on the Boltzmann equation. Good agreement is found between the numerical results and a recent analytic solution under a relaxation-time approximation for electron-phonon scattering [S. K. Lyo, Phys. Rev. B 77, 195306 (2008)]. Different roles played by elastic and inelastic scattering on the damped Bloch oscillations and the nonlinear steady-state are demonstrated from our numerical results. We will also briefly discuss suppression of the dynamical localization by strong Bloch oscillations under an additional nonlinear AC field and opposite roles played by elastic and inelastic scattering on the damped dynamical localization.

3:30PM D21.00006 Full Counting Statistics of a Quantum Point Contact with Time-dependent Transparency, JIN ZHANG, YURY SHERKUNOV, NICHOLAS D’AMBRUMENIL, BORIS MUZYKANTSKII, Department of Physics, University of Warwick — Controlled injection of single electrons into a ballistic conductor is essential for “moving-electron-based” quantum computation. We consider an electron system in two 1D ballistic conductors separated by a tunneling barrier at zero temperature. We present numerical results for the full counting statistics (FCS) for the case when the barrier potential is modulated in the presence of a time-dependent bias voltage applied between the leads. The calculation is based on Abanov and Ivanov’s formula[1]. For the case of a periodic input with a large number of cycles, we perform the calculation in discretized energy space and obtain the characteristic function $\chi(\lambda)$ as well as physical observables such as the current, noise and entanglement entropy directly. We show how to optimize the gate potential of a quantum point contact to generate a single electron excitation with minimal noise. [1]A.G. Abanov and D.A. Ivanov, Phys.Rev.Lett., 100, 086602.

3:42PM D21.00007 Optimal electron entangler at low temperatures, YURY SHERKUNOV, JIN ZHANG, NICHOLAS D’AMBRUMENIL, BORIS MUZYKANTSKII, University of Warwick — Electron transport in mesoscopic contacts at low temperatures is accompanied by logarithmically divergent equilibrium noise when a tunneling barrier transparency is changed abruptly. We show that the equilibrium noise can be dramatically suppressed in the case of tunneling junction with smoothly tunable transparency. We study analytically the full counting statistics of the transparency modulated quantum contact and identify the minimal excitation states generated by the gate voltage. The proposed scheme could be used as an optimal electron entangler at low temperatures.
3:54PM D21.00008 Observation of quantum phase shift in an Aharonov-Bohm ring with a fully controlled flying charge qubit, MICHIHISA YAMAMOTO, Department of Applied Physics, University of Tokyo, CHRISTOPHER BAUERLE, Institut Neel, CNRS, SEIGO TARUCHA, Department of Applied Physics, University of Tokyo, and ICPP-R-JST — Aharonov-Bohm effect is one of the most typical interference phenomena of electrons. Although a number of experiments have been performed to date, observation of phase shift at each path has been rather difficult due to the phase rigidity in the two-terminal setup. In this study, we employed a hybrid device consisting of a parallel coupled-wire and an AB ring, in which each coherently propagating electron acts as a flying qubit. In this device, phase rigidity no longer exists as there are two output contacts. The qubit is defined as superposition of two quantum states: an electron exists in one of the two wires. Then, the inter-wire tunnel coupling gives flipping between the two quantum states, and the evolution of the phase in the AB ring is translated into rotation about the z-axis of the Bloch sphere. In the experiment, we define the initial qubit state by injecting electrons into only one of the two wires, and obtained the arbitrary output state by tuning gate voltages. The output state also oscillates as a function of perpendicular magnetic field $B$ with the AB oscillation period. We observed the shift of k-vector in one of the two wires works equivalently as the shift of off. This is the direct observation of the phase shift $\Delta \phi = \Delta k l$.

4:06PM D21.00009 Current dependent dephasing in an Aharonov-Bohm Interferometer, KUAN-TING LIN, YIPING LIN, J. C. CHEN, Department of the Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, T. UEDA, S. KOMIYAMA, Department of Basic Science, University of Tokyo, Komaba, Tokyo 153-8902, Japan — We have studied the temperature dependence of the current induced dephasing in a ballistic GaAs/AlGa$_x$As ring. The dephasing rate is linearly proportional to the temperature regardless of the current applied. The AB oscillations are suppressed by the increase of the excitation current; however, the dephasing becomes less temperature dependent. Our observations cannot be interpreted by Joule heating effect. Possible decoherence mechanisms caused by the excess current will be discussed.

4:18PM D21.00101 Tumbale Channel Interference in an Aharonov-Bohm Ring, YIPING LIN, PEI-JUNG WU, KUAN-TING LIN, J. C. CHEN, Dep. of Physics, National Tsing Hua University, Hsinchu, Taiwan, T. UEDA, S. KOMIYAMA, Dep. of Basic Science, University of Tokyo, Meguro-ku, Tokyo, Japan — We have investigated the Aharonov-Bohm effect in a quasi one-dimensional ring on a GaAs/Al$_{0.3}$Ga$_{0.7}$As heterostructure fabricated by two metallic arc deposition and shows only a 6% variation of the temperature dependence of the channel width of electrons, thereby externally tuning the transverse modes in the interference paths. The oscillatory magnetoconductance of the device is systematically studied by varying the number of channels in each path. We have observed the evidence of phase shifts in the magnetoconductance oscillations due to the suppression of the mode numbers on the ring path. Though the periodicity is not well resolved, qualitatively our data support the random phase shifts between the successive modes.

4:30PM D21.00111 Transport and noise in 90nm n-GaAs Epilayers, A. GILBERTSON, J.D. MOORE, G. PERKINS, J. GALLOP$^2$, L.F. COHEN, Imperial College, A.K.M. NEVIAZ, S.A. SOLIN$^3$, Washington University — Extraordinary Magnetoresistance (EMR) belongs to the family of EXX effects which form the basis for a number of devices that offer the potential for high sensitivity applications. Such devices would benefit from minimising the active volume of the sensor. To reduce that volume and minimize wafer fabrication complexity it is desirable to employ uni-tran-GaAs epilayers. Accordingly, we report here the transport and noise properties of 90nm Si-doped GaAs films grown by molecular beam epitaxy which have been fabricated into both microscopic EMR devices and macroscopic van der Pauw geometries. These films exhibit a room temperature electron mobility and density of 3225 cm$^2$/V s$^{-1}$ and 1.45x10$^{17}$ cm$^{-3}$, respectively, and shows only a 6% variation of the temperature dependence of the channel width of electrons, thereby externally tuning the transverse modes in the interference paths. The oscillatory magnetoconductance of the device is systematically studied by varying the number of channels in each path. We have observed the evidence of phase shifts in the magnetoconductance oscillations due to the suppression of the mode numbers on the ring path. Though the periodicity is not well resolved, qualitatively our data support the random phase shifts between the successive modes.

4:42PM D21.00012 New Measurement of Diffusion Thermopower of 2D Electron Systems, W.E. CHICKERING, J.P. EISENSTEIN, Caltech, J.L. RENO, Sandia — The thermoelectric properties of low-dimensional electronic systems provide information about carrier transport that is complementary to that obtained from charge transport and determined relatively easily. In conventional measurements of the thermopower $S$ of two-dimensional electron systems (2DEGs), phonon drag overcomes the diffusion thermopower $S_d$ of the electron gas for temperatures $T > \sim 0.1$ K. We introduce a new hot electron thermocouple technique which vastly reduces the importance of phonon drag and allows us to accurately determine $S_d$ in a 2DES in a GaAs/AlGaAs heterostructure. Differentialley gated 2DES channels provide the analogs of the dissimilar metals used in a conventional thermocouple. The device is calibrated via the temperature dependence of the longitudinal resistance of the 2DES at the thermocouple junction. Our results are in good quantitative agreement with the Mott formula for the temperature dependence of $S_d$ for temperatures up to $T \sim 2$ K. This work is supported by DOE grant DE-FG03-99ER45766 and Microsoft Project Q.

4:54PM D21.00013 Thermopower of n- and p-type InN, NATE MILLER, Lawrence Berkeley National Lab, Univ. of California - Berkeley, JOEL AGER, Lawrence Berkeley National Lab, REBECCA JONES, HOLLAND SMITH, Lawrence Berkeley National Lab, Univ. of California - Berkeley, LADEK WALUKIEWICZ, Lawrence Berkeley National Lab, WILLIAM SCHAFF, Cornell University, CHAD GALLINAT, GREGOR KOBLMULLER, JIM SPECK, Univ. of California – Santa Barbara — The exceptionally large (\textgreater{} 5.5 ev) electron affinity of InN leads to unique electronic properties such as surface electron accumulation and an extreme propensity for n-type conduction. This, combined with a small energy gap and strongly energy dependent effective mass, makes an analysis of charge transport and determination of band structure parameters an arduous task. In this work we show that thermopower (Seebeck coefficient) measurements can address some of the issues by providing a new tool to study the unique charge transport properties of InN and In-rich group III-nitride alloys. Our thermopower experiments are used to demonstrate the presence of mobile holes in Mg-doped InN providing the first direct, quantitative measurement of hole transport in InN. We also report modeling of the thermopower of n-type InN considering the various scattering mechanisms.

5:06PM D21.00014 Measurement of [N] and T-dependence of electron effective mass in GaAsN, TASSILIO DANNECKER, Tyndall National Institute, YU JIN, Materials Science and Engineering, University of Michigan, JOHN BUCKERIDGE, Tyndall National Institute, CITTERAU UHER, CAGLIYAN KURDAK, Physics Department, University of Michigan, STEPHEN FAHY, Tyndall National Institute, RACHEL S. GOLDMAN, Materials Science and Engineering, University of Michigan — The electron effective mass of GaAs$_{1-x}$N$_x$ is predicted to be dependent on N-composition, $x$, and temperature, $T$; however, conflicting results have been observed using cyclotron resonance and thermomagnetic measurements. Using thermopower and Hall measurements, in conjunction with assumptions of parabolic bands and Fermi-Dirac statistics, we determined the T-dependence of the electron effective mass of GaAs$_{1-x}$N$_x$, in comparison with that of GaAs. Measurements of the T-dependent Seebeck coefficient, $S$, for N compositions ranging from $x=0$ to 0.0100, reveal a decrease in $\Delta S$ with $x$. For GaAs, the free carrier concentration, $n$, is independent of $T$. In all other cases, $n$ increases (decreases) with $T$. For GaAsN, the effective mass decreases from 0.06$\mu_0$ at 140K to 0.052$\mu_0$ at 300K, similar to literature reports. For GaAsN, the effective mass approximately decreases (increases) with $x$ and $T$, ranging from 0.18$\mu_0$ to 0.16$\mu_0$ at 140K, with values 14% (40%) lower for $x=0.0075$ ($x=0.0100$) at 300K.
5:18PM D21.00015 Temperature dependence of electron mobilities in InN\(^1\). LEONARDO HSU, University of Minnesota, WLADIMIR WALUKIEWICZ, Lawrence Berkeley National Laboratory — InN allows the possibility of engineering nitride materials with bandgaps as small as 0.7 eV. We have calculated electron mobilities in InN taking into account the non-parabolicity of the conduction band, as well as the standard scattering mechanisms of acoustic and optical phonons and Coulomb scattering from charged impurities. Although our calculations explain well the experimentally measured mobilities at temperatures higher than about 200 K, the measured mobilities in lightly doped InN at low temperatures decrease in a way that cannot be accounted for by the standard theory. We discuss the characteristics and possible origins of the additional mechanism that must be included in the calculations in order to fit the experimental results.

\(^1\)This work was partially supported by the US DOE under Contract No. DE-AC03-76SF00098.

Monday, March 16, 2009 2:30PM - 5:18PM —
Session D22 GMAG DMP FIAP: Focus Session: Spins in Group IV Semiconductors 324

2:30PM D22.00001 Quantum control of donor electron charge and spin in Si close to a Si-SiO\(_2\) interface. BELITA KOILLER\(^1\). Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil — Doped Si is a promising candidate for quantum information processing due to its potential for scalability, long spin coherence times, and the continuing progress on Si material processing, technology and miniaturization over several decades. I will discuss important issues for single- and two-qubit operations in Si-based quantum computer proposals involving P donors close to a SiO\(_2\) interface. For a single donor, bound-orbital electron manipulation between the donor and the interface by electric and magnetic fields is investigated [1,2]. Valley interference and how it affects a donor electron close to an interface under an applied electric field is also considered, taking the valley-orbit coupling at the interface as a parameter. It will be shown that, for nonzero interface valley-orbit coupling, this configuration leads to oscillatory behavior of the donor ionization time as a function of the donor-interface distance while the characteristic ionization field does not oscillate with distance [3]. The physical origin of these effects, and their impact in proposed operations of donor-based qubits, will be discussed. For a donor pair, the exchange coupling of interface electrons bound to the donors double well potential is calculated within the Heitler London approach [2,4]. The feasibility and convenience of performing exchange operations for electron pairs at the interface as opposed to around the donors will be assessed. Work done in collaboration with M.J. Calderon and S. Das Sarma and partially supported by LPS-NSA and MICINN-Spain.


1Support by the Brazilian agencies CNPq, FAPERJ and Instituto do Milenio de Nanotecnologia-MCT

3:06PM D22.00002 A new electrical readout mechanism for Si:P qubits. DANE R. MCCAMEY, University of Utah, G.W. MORLEY, London Centre for Nanotechnology, S.-Y. PAIK, S.-Y. LEE, University of Utah, L.-C. BRUNEL, University of California, Santa Barbara, J. VAN TOL, National High Magnetic Field Laboratory, C. BOEHME, University of Utah — Phosphorus donor spins in silicon are a promising candidate for the implementation of quantum bits, and electrical detection is viewed as the most promising route towards the single donor readout required to further advance such concepts. We will discuss a major limitation to commonly used electrical detection schemes. The standard way to electrically detect Si:P spin states involves utilizing spin dependent recombination with nearby probe spins, usually of defects at the Si-SiO\(_2\) interface. This process has a fast, fixed timescale, thereby limiting coherence times. We find that these times are of order 1\(\mu\)s, in agreement with other studies. By moving to high magnetic fields (\(B > 8 \text{T}\)) we enter a new regime - complete electron polarization. This allows us to utilize a different readout mechanism, namely, capture into the donor D\(^-\) state which causes a decrease in the photocurrent in the sample. We have developed a system which allows us to investigate the donor spin phase coherence times at these high magnetic fields; we find them to be over 100\(\mu\)s [1]. Additionally, the signal observed at these high fields is significantly larger (\(\Delta I/I \sim 5\%\)) than at low fields, providing a pathway towards single spin detection. [1] PRL 101, 207602 (2008)

3:18PM D22.00003 SU(4) Kondo in a single donor transport in a Si FinFET. G.P. LANSBERGEN, G.C. TETTAMANZI, A. VERDUIJN, M. BLAUBOER, S. ROGGE — Recently, single dopants became experimentally accessible and there is a large effort to exploit their atomic characteristics in nano devices. Orbital Kondo effects in Si and SiGe are of fundamental interest since they explore the role of the valley degree of freedom in this material system. It has been theoretically predicted that the valley degeneracy leads to SU(4)-correlations which entangles the spin and momentum of exchanged electrons. Here, we experimentally study Kondo effects in a novel system, a single shallow donor in a three-terminal geometry. We use Si wrap-around gate (FinFET) devices with a single Arsenic donor atom in the channel dominating the sub-threshold transport characteristics. The ground state of this system originates from the hybridization of the donor hydrogen-like state which has no valley degeneracy (due to the strong valley-orbit interaction) and a quantum dot-like state which is two-fold valley degenerate. In the Coulomb-blockade regime with a single electron on the system we observe a set of transport resonances. We show these resonances to originate from Valley Kondo effects by means of their dependence on temperature, magnetic field, orbital splitting and their substructure. The entanglement between spin and momentum provides new opportunities for spin control in silicon. For example, we show that this device operates as a gated spin filter in Si with a potentially high transitivity.

3:30PM D22.00004 Electric field control of spins in a silicon two-dimensional electron gas. R. JANSEN, B.C. MIN, S. P. DASH, R. S. PATEL, M. P. DE JONG, University of Twente, MESA+ Institute for Nanotechnology, The Netherlands — A key objective in the development of semiconductor spintronics is the active control of spins in semiconductors. The manipulation by electric rather than magnetic fields is preferred as this is more efficient for nanoscale high frequency devices. Proposals for electric spin control, for example in use in a spin transistor, have so far focused on mechanisms that require spin-orbit interaction. Unfortunately, in silicon, the mainstream semiconductor, the weak spin-orbit interaction renders these mechanisms unsuited. Hence, alternative approaches are paramount to the success of semiconductor spintronics. Here we demonstrate spin control by electric fields in a silicon two-dimensional electron gas (2DEG), exploiting the discrete electronic structure of the 2DEG. This, in combination with an electric field, allows spin manipulation without the need for spin-orbit interaction. The spin control is manifested as resonances in the tunnel magnetoresistance between the Si 2DEG and a ferromagnetic tunnel contact, with amplitude of up to 8%.
3:42PM D22.00005 Injection and extraction of spins in a Silicon lateral transport structure . OLAF VAN 'T ERVE, CHAFFRA AWO-AFFOUDA, AUBREY HANBICKI, MICHAEL HOLUB, CONNIE LI, PHILLIP THOMPSON, BÉRENDE JONKER, Naval Research Laboratory, NAVAL RESEARCH LABORATORY TEAM — Significant progress has recently been made on spin injection into the technologically important semiconductor, Si. A nonlocal measurement technique, which excludes spurious contributions from AMR and local Hall effects, was used to show lateral diffusive spin transport through silicon using Fe/Al2O3 surface contacts. The tunnel contacts are used to create and analyze the flow of pure spin current in a silicon transport channel. The nonlocal signal shows that a spin current can be electrically detected after diffusive transport through the silicon transport channel and the signal depends on the relative orientation of the magnetization of the injecting and detecting contacts. Hanle effect measurements up to 125 K demonstrate that the spin current can be modulated by a perpendicular magnetic field, which causes the electron spin to precess and dephase in the channel during transport. By changing the bias on the injector contact we can either inject or extract spin from the Silicon channel. Here we will show using Hanle and lateral spin-valve measurements that we can change the polarization of the spin accumulation by going from the injection regime to the extraction regime and we will compare the efficiency of spin-injection versus spin extraction.

3:54PM D22.00006 Spin Precession in Oblique Magnetic Fields . JING LI, BIQIN HUANG, Department of Electrical and Computer Engineering, University of Delaware, IAN APPELBAUM, Department of Physics, University of Maryland, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, UNIVERSITY OF DELAWARE TEAM — Spin precession and dephasing (“Hanle effect”) provide an unambiguous means to establish the presence of spin transport in semiconductors. We compare theoretical modeling with experimental data from drift-dominated silicon spin transport devices, illustrating the non-trivial consequences of employing oblique magnetic fields (due to misalignment or intentional, fixed-in-plane field components) to measure the effects of spin precession. Model results are also calculated for Hanle measurements under conditions of diffusion-dominated transport, revealing an expected Hanle peak-widthing effect induced by the presence of fixed-in-plane magnetic bias fields.

4:06PM D22.00007 Geometric dephasing-limited Hanle effect in long-distance lateral silicon spin transport devices . BIQIN HUANG, HYUK-JAE JANG, University of Delaware, IAN APPELBAUM, University of Maryland — Using ballistic injection and hot-electron spin filter detection, lateral spin transport over 2 millimeters is demonstrated in undoped single-crystal Silicon. In these devices, geometrically-induced dephasing (Hanle effect) is so strong that the effects of spin precession could not be measured with only a single-axis magnetic field. However, a two-axis magnetic field can be used to obtain unequivocal evidence of spin precession and transport despite full dephasing. We therefore conclude that there is never a reason to avoid measurement of spin precession as unequivocal evidence of spin transport in semiconductor devices.


4:30PM D22.00009 Indirect Optical Injection of Carriers and Spin in Silicon . JINLUO CHENG, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, JULIEN RIOUX, JOHN SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto — Degenerate two-photon indirect absorption in silicon is an important limiting effect on the use of silicon structures for all-optical information processing at telecommunication wavelengths. Optical injection of spins in silicon is potentially important for spintronics applications. We theoretically investigate one- and two-photon indirect absorption in silicon, using a pseudopotential description of energy band and the adiabatic bond charge model to describe phonon dispersion and polarization. Spin injection is calculated as well. We compare our results with experiments.

4:42PM D22.00010 Transient Current Spectroscopy of a Si Quantum Dot . MING XIAO, HONGWEN JIANG, UCLA — We present a transient current spectroscopy study of a Si-MOS based quantum dot. The study was conducted in the few electron region. A voltage pulse pumps the electrons into an excited orbital state and the non-equilibrium transient current through the dot was recorded. The evolution of the excited state as a function of magnetic field shows signatures of a transition from a spin singlet state to a triplet state of an electron pair. A pump-and-probe technique was employed to set a lower limit of the triplet-singlet relaxation time. The work was sponsored by United States Department of Defense.

4:54PM D22.00011 Magneto-transport properties of Bi-based Nanowires . SUNGMU KANG, JUGDERSUREN BATTGGOTOKH, ANDREW C. BUCHELE, DAVID A. MCKWEO, IAN L. PEGG, JOHN PHILIP1, Catholic University of America, VITREOUS STATE LABORATORY COLLABORATION — We report the growth and magneto-transport properties of Bi-based, Mn$_3$SiC nanowires grown using chemical vapor deposition. High resolution transmission electron microscopy and x-ray diffraction studies show that the nanowires crystallize in Mn$_3$SiC orthorhombic structure. Ferromagnetic Mn$_3$SiC nanowires were grown using a coordination complex-based precursor. In the presence of an external magnetic field, Mn$_3$SiC nanowire-based devices exhibit spin dependent transport at room temperature. A large change in current with almost two orders of magnitude increase is observed when a small field is applied parallel to the axial direction of the nanowire. We will discuss in details the magneto-transport properties of Mn$_3$SiC nanowire based devices.

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5:06PM D22.00012 Prospects of Spin Injection in Germanium Nanowires . EN-SHAO LIU, KAMRAN VARAHRAMYAN, JUNGYO NAH, SANJAY BANERJEE, EMANUEL TUTUC, Microelectronics Research Center, University of Texas at Austin — Efficient spin injection from ferromagnetic (FM) contacts into semiconductors (SC), the prerequisite for spin-based semiconductor devices, is typically suppressed by the conductivity mismatch between the FM contact and the SC. A significant spin injection can be achieved however if the contact resistivity at the FM/SC interface is appropriately engineered [1]. We report here contact resistivity measurements of n-type germanium (Ge) nanowires (NWs) with two FM metals, namely permalloy (Ni$_{80}$Fe$_{20}$) and nickel (Ni), for NW doping densities between $10^{16}$ and $10^{20}$cm$^{-3}$, and for temperatures between 77K to 300K. Using back-gated two- and four-terminal measurements, we show that the contact resistivity varies from $10^{-2}$($\Omega \cdot \text{cm}$) for highly-doped NWs, to $10^{-4}$($\Omega \cdot \text{cm}$) for moderately-doped NWs. Within the framework of the spin injection theory [1], these values indicate that by optimizing the device parameters, namely the choice of FM metal, contact width, NW diameter and doping density, spin injection into Ge NWs is possible. [1] A. Fert and H. Jaffres, Phys. Rev. B. 64, 184620 (2001)
Monday, March 16, 2009 2:30PM - 5:30PM –
Session D23 DCMP: Diffusion and Transport Properties 325

2:30PM D23.00001 A multiscale study of hydrogen embrittlement of metals: Revisiting the hydrogen enhanced local plasticity (HELP) mechanism. JOHANN VON PEZOLD, JÖRG NEUGEBAUER, Max Planck Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — The embrittlement of metals by H is a long-standing problem, whose underlying mechanisms are still largely unclear. Here we consider the atomistic basis of the HELP mechanism, which asserts that H mobilises dislocations by shielding elastic dislocation-dislocation interactions. Using a combination of density-functional theory calculations, semiempirical EAM potentials and an effective lattice gas Hamiltonian we determine the interaction of H with the strain field around edge dislocations in Ni. Our results reveal an attractive, but short ranged interaction between H interstitials, which leads above a critical concentration to the formation of a precursor hydride phase. The increased lattice parameter of this hydride phase induces significant misfit stress, but localises the dislocation stress field due to a localisation of the dislocation strain field. For H concentrations of up to 0.25 at. %, the stress localisation is found and thus effectively shields the stress field of the dislocation, pointing towards a novel atomistic basis for the HELP mechanism.

2:42PM D23.00002 DFT energetics of hydrogen binding to point defects in iron and steels. WILLIAM COUNTS, CHRIS WOLVERTON, RON GIBALA, Northwestern University — It is well known that hydrogen degrades the properties of iron and steel. One proposed mechanism of hydrogen attack is the concept of "hydrogen traps", which are generally microstructural material defects that bind hydrogen atoms. The stability and energetics of a number of potential traps (like vacancies, interstitials, and substitutional alloying elements) in bcc and fcc iron are investigated using density functional theory (DFT). We find that hydrogen is very sensitive to its local environment. For example, in a perfect bcc iron lattice, hydrogen prefers to sit in the tetrahedral site rather than the octahedral site or a substitutional site, and there is a repulsive interaction between carbon and hydrogen. In the presence of a vacancy, the energy barrier between the octahedral and tetrahedral sites disappears and hydrogen only resides in the octahedral sites. The hydrogen-vacancy binding energy changes as more hydrogen atoms bind to the vacancy, but the binding energy does not significantly change in the presence of carbon. We also find that H2 molecules are not stable inside a vacancy: they dissociate spontaneously (without a barrier) into octahedral positions. Details about vacancy and other potential traps are presented and their roles in hydrogen embrittlement are discussed.

2:54PM D23.00003 First-principles studies of helium in palladium tritides: PdT3 = (0 ≤ x ≤ 1). PEI LIN, YAN WANG, M.Y. CHOU, School of Physics, Georgia Institute of Technology — Helium bubbles have significant impact on the stability and mechanical properties of materials used in nuclear-energy systems. Theoretical studies on the behavior of H in various metals have been reported in the past. However, few studies have taken into account the effect of the coexistence of He and tritium (3H) in the metal lattice. We have performed first-principles calculations of He inside palladium tritides with various H concentrations. Instead of interacting with He impurities directly, the interstitial H mainly modifies the electronic structure of the metal lattice. The Pd d-orbital near the Fermi-level shifts downward as H atoms occupy the interstitial sites, which in turn promotes the interaction between He 2-s and Pd 4-d states. We have examined the changes in the formation energy of an He impurity with various H concentrations. The effect will further modify the energetics of trapping multiple He atoms to form a cluster inside the hydrogenated Pd system.


3:18PM D23.00005 Prediction and Modeling of Atomic Mobility in Alloys, ZI-KUI LIU, Department of Materials Science and Engineering, The Pennsylvania State University — Atomic diffusion is a common and important non-equilibrium process in solids that takes place at finite temperatures. To computationally simulate atomic diffusion processes, the thermodynamic and atomic mobility databases of the materials of interest are needed. The modeling technique of atomic mobility databases and related software has been becoming more and more matured in the last decades. However, the input data for the modeling is exclusively taken from experimentally measured tracer and chemical diffusion coefficients. In this presentation, our recent progress in predicting self and dilute diffusion coefficients by quantum mechanics calculations will be discussed [1]. Our approach to the unstable vibrational mode of transition states during diffusion will be presented. The contribution to phenomenological modeling of atomic mobility will be briefly.

3:30PM D23.00006 Analysis of Cd jump rates among the two Ga sublattices in Ga2-Pd3 using a stochastic model of hyperfine interactions. , M. O. ZACATE, Northern Kentucky University, Highland Heights, KY, W. E. EVENSON, Utah Valley University, Orem, UT, G. S. COLLINS, Washington State University, Pullman, WA — Atomic jump rates of Cd among the two inequivalent Ga sublattices in Ga2-Pd3 were measured using perturbed angular correlation spectroscopy (PAC). Atomic jumps result in a reorientation and/or change in strength of electric field gradients experienced by the Cd PAC probes. Spectra were fitted to model functions generated using a stochastic model for fluctuating EFGs under the assumption that Cd probes can jump to nearest neighbor sites of each Ga sublattice. Jump activation energies were determined by fitting spectra collected at different temperatures simultaneously under the constraint that jump rates obey Arrhenius behavior. The following activation energies were determined for intra-sublattice jumps: 0.52(1) eV for Ga(3)→Ga(3) and 0.25(4) eV for Ga(4)→Ga(4) and for inter-sublattice jumps: 0.6(3) eV for Ga(3)→Ga(4) and 0.47(9) eV for Ga(4)→Ga(3), in which Ga(4) denotes the site with .3m point symmetry.

3:42PM D23.00007 Vanadium diffusion in ferrite, SUNGHO KIM, JEFFREY HOUZE, SEONG-GON KIM, MARK HORSTE-MEYER, Mississippi State University — Vanadium is a very important additive in high strength steel alloys. Small amount of vanadium addition strengthens the steel alloys. As a first step to study the effect of vanadium addition in steel alloys we calculated the diffusion path and the migration energy of vanadium atom in ferrite crystal using first principles calculations.
3:54PM D23.00008 Anisotropic physical properties of RSn2 (R = Gd - Lu) single crystals, EMILIA MOROSAN, MICHAEL MEHLMAN, LIANG ZHAO, THOMAS SANDERS, Physics and Astronomy, Rice University — A wealth of magnetic and electronic properties (including metamagnetism, spin glass, non Fermi liquid behavior etc) has been observed in rare earth intermetallic compounds. The availability of these systems in single crystal form is imperative for characterizing their complex behavior. We are reporting the anisotropic physical properties of single crystals of the orthorhombic RSn2 compounds (R = Gd - Lu). Complex anisotropic H-T phase diagrams are observed in GdSn2, which has an antiferromagnetic ground state below 27.5 K, with two more transitions at lower temperatures. The magnetic field induces magnetostatic phase transitions in several of the R members of the series.

4:06PM D23.00009 Mesostructural properties of RCO2 (R = rare earth) compounds1, DURGA PAUDYAL, YA. MUDRYK, Ames Laboratory of the USDOE, Iowa State University, Ames, IA-50011, V. K. PECHARSKY, K. A. SCHNEIDER, JR., Ames Laboratory of the USDOE and Department of Materials Science and Engineering, Iowa State University, Ames, IA-50011 — First principles electronic structure calculations show that the cubic Laves phase (C15) is stable for GdCO2 and TbCO2, while the ground state structures of DyCO2, HoCO2, and ErCO2 are tetragonal distortions of the cubic C15, orthorhombic, and rhombohedral structures, respectively. The R and Co moments exhibit antiparallel coupling, forming a ferrimagnetic state in every monomorphic ground state structure of RCO2. The predicted mesostructural properties of RCO2 are in good agreement with x-ray powder diffraction and magnetic measurements. The spin splitting of the conduction electrons due to the indirect R-R exchange plays a crucial role in the mesostructural transformations in the R = Dy, Ho, and Er RCO2 phases, and accounts for its absence in the monomorphic GdCO2 and TbCo2 compounds.

1This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under contract No. DE-AC02-07CH11358 with Iowa State University of Science and Technology.

4:18PM D23.00010 Transition in NiMnSn and NiMnIn, C.P. OPEIL, Boston College, J.C. LASHLEY, J.L. SMITH, Los Alamos National Laboratory, T. PLANES, L. MANOSA, University of Barcelona — Magneto-transport, specific heat, magneto-striction and temperature dependent UV photoemission are used to explore the martensite transition of the ferromagnetic shape memory alloys Ni2MnIn2, Ni2MnIn2Sn2. Comparisons will be made to a previous work on the stoichiometric single crystal Ni2MnGa which reveals a temperature (T ≥ 190 K) and field dependent (0 – 1 T) positive/negative magneto-resistance slope. Our experimental results will be discussed in light of a possible pseudo-gap formation coincident with the martensite transition in the two off-stoichiometric alloys.

4:30PM D23.00011 Measurements of persistent currents in normal metal rings with cantilever torsional magnetometry, WILLIAM SHANKS, ANIA BLESZYNSKI JAYICH, BRUNO PEAUDECERF, JACK HARRIS, Department of Physics, Yale University — We have measured the magnetization of arrays of micron-scale aluminum rings at low temperatures and in high magnetic fields using cantilever torsional magnetometry. We see clear evidence of normal state persistent currents in these rings. The current’s dependence on magnetic field, temperature and the rings’ circumference is consistent with theoretical predictions (due to Riedel and von Oppen) for non-interacting electrons in the diffusive regime. To fully characterize these samples, we also measured the magnetization of codeposited rings in the superconducting state and the magnetoresistance of codeposited wires. Together these measurements provide an especially clear picture of the normal-state persistent currents.

4:42PM D23.00012 ABSTRACT WITHDRAWN —

4:54PM D23.00013 AC-conductance of a quantum chaotic cavity (semiclassical approach)1, C. PETITJEAN, D. WALTNER, J. KUIPERS, I. ADAGIDELI, K.R. RICHTER — Due to the progress made in the control and the manipulation of mesoscopic structures driven by high frequency periodic voltages, the ac regime has been recently experimentally investigated [1] and consequently its theoretical interest has been renewed. We consider here, a quantum chaotic cavity that is coupled via tunnel barriers and gates to a macroscopic circuit which contains ac-sources [2]. By extending to the ac-transport, the recent trajectory-based semiclassical theory of quantum chaotic transport in presence of tunnel barrier [3], we derive for arbitrary tunneling rates and arbitrary positive Ehrenfest time, the averaged and the weak-localization correction to the screened conductance. Then we use these results to investigate the effect of dephasing on the relaxation resistance of a chaotic capacitor in the linear low frequency regime. This last investigation is of prime importance as it is very close to the recent measurement of the admittance at zero magnetic flux of a mesoscopic capacitor [1,4].

References:

1Funded by the Alexander von Humboldt foundation.

5:06PM D23.00014 ABSTRACT WITHDRAWN —

5:18PM D23.00015 Evidence for Conditioning as a Progenitor of Double-C Transformation Mechanisms in Pu-Ga Alloys1, J.R. JEFFRIES, K.J.M. BLOBAUM, M.A. WALL, A.J. SCHWARTZ, Lawrence Livermore National Laboratory — By alloying Pu with Ga, the fcc δ phase can be retained down to room temperature. This metastable δ phase is realized due to slow Ga diffusion, which prevents the δ phase from decomposing into the equilibrium mixed phase structures. The metastable δ phase in a Pu-1.9 at.% Ga alloy, however, does yield to chemical driving forces by undergoing the δ → α' isothermal martensitic transformation below Mα' ≈ -100 °C. This transformation exhibits poorly understood double-C behavior in the time-temperature-transformation diagram. Recently, a “conditioning” treatment—which entails isothermally holding a specimen at sub-annal temperatures but above Mα' —has been shown to dramatically affect the amount of α' phase formed at low temperature. We report evidence that the conditioning treatment induces the lower-C of the double-C curve, and we implicate the classical nucleation of equilibrium phases as the underlying mechanism behind conditioning in Pu-Ga alloys.

1Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under Contract DE-AC52-07NA27344.

Monday, March 16, 2009 2:30PM - 5:18PM –
Session D24 DMP: Focus Session: Nanotube manipulation and processing 326
2:30PM D24.00001 Carbon nanotube devices: Sorting, Assembling, Characterizing  
RALPH KRUPKE, Forschungszentrum Karlsruhe — Carbon nanotubes have been studied extensively over the last decade. Various exceptional properties have been revealed which still drive the vision about using carbon nanotube in future electronics, for instance as molecular nanoscale transistors or electromigration resistant interconnects. For many years a major obstacle was the inability to grow nanotubes with defined dimensions (length, diameter) and electronic properties (metallic, semiconducting). Recently these problems have been solved to a large extent by advanced sorting techniques. Today the challenge is to assemble nanotubes devices with defined properties to form a complex circuit. As progress is made in making highly-integrated nanotube device arrays new characterization techniques have to be developed which allow testing large number of devices within an acceptable time. Along this line I will report on the state-of-the-art of sorting of carbon nanotube, as a base for nanotube device fabrication [1]. I will then explain our strategy to assemble high-density arrays of nanotube devices [2] and discuss a new characterization technique for nanotube devices [3]. Finally I will introduce a novel device engineering tool [4].


3:06PM D24.00002 Self-healing and adsorbate-induced removal of defects on graphene and carbon nanotubes  
LEONIDAS TSETSERIS, Vanderbilt University and University of Thessaloniki (Greece), SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The presence of point defects is known to induce significant changes in the electronic, chemical, transport, and mechanical properties of graphitic systems. Here, we use first-principles calculations based on density-functional theory to describe several adatom-related processes that alter key physical traits of graphene and carbon nanotubes. We find that, while pairs of C adatoms and clusters of four or more self-interstitials stay idle unless the system is heated to very high temperatures, clustering of three C adatoms leads to removal of hillock-like features and creates mobile species, resulting in self-healing of defective structures. We also demonstrate the reactivity of defect pairs using hydrogen and oxygen as prototype adsorbates, and we show that interaction with extrinsic species is an alternative healing mechanism for adatom structures in the above systems. The results relate to the evolution of defects either during growth of carbon nanotubes or during post-growth treatment and operation of related devices. This work was supported in part by DOE Grant DEFG0203ER46096.

3:18PM D24.00003 Self-similar mechanics of vertically aligned carbon nanotube organization  
MICHAEL DE VOLDER, SAMEH TAWFICK, DANIEL VIDAUD, A. JOHN HART, University of Michigan — It is well-known that carbon nanotube (CNT) growth from a dense arrangement of catalyst nanoparticles creates a self-organized vertically aligned CNT “forest” that offers attractive anisotropic mechanical, thermal, and electrical properties. Self-organization is governed by the CNT diameter and spacing, and the surface interactions between contacting CNTs. We demonstrate that arrays of CNT microstructures having micron-scale diameter organize in a similar manner as individual CNTs within a forest. For example, as postulated for forest CNTs, entanglement of CNT microstructures during the initial stage of growth creates a self-supporting network, and this enables coordinated subsequent growth of the structures in the vertical direction. The alignment of these self-similar CNT forests is inversely related to the spacing of the individual CNTs, and like individual CNTs, widely-spaced microstructures that are not self-supporting fail to organize into an oriented superstructure. The growth rate and final forest height also depend on these geometric conditions, suggesting that mechanical interactions affect the collective progression and termination of a CNT film. This study and method offers new insights into the self-organization of one-dimensional nanostructures, and coordinated assembly of CNT microstructures offers opportunity for engineering energy-absorbing foams and photonic crystals.

3:30PM D24.00004 Debundle of Single-Walled Carbon Nanotubes with Exfoliated Nanoplatelets1, DAZHI SUN, WILLIAM EVERETT, CHIEN-CHIA CHU, HUNG-JUE SUE, Texas A&M University, PROF. SUE'S TEAM — We report a simple and effective colloid method to disperse single-walled carbon nanotubes (SWNTs) down to individual-tube level by utilizing exfoliated nanoplatelets in various solutions and polymer matrices. This approach yields a substantial amount of individual tubes without compromising their physical properties. The de- bundling and dispersion of SWNTs are confirmed by high-resolution transmission electron microscopy, UV-vis-NIR and Raman spectroscopy. After incorporated into polymers, SWNTs maintain individual dispersion. The dispersion mechanisms and implications of this approach are also discussed.

1We thank Kaneka and Defense Logistic Agency (SP0103-02-D-0003) for their partial financial support of this research.

3:42PM D24.00005 Motion and Manipulation of Suspended Single-Walled Carbon Nanotubes in Solution  
YA-QIONG XU, Laboratory of Atomic and Solid State Physics, Cornell University, ARTHUR BARNARD, School of Applied and Engineering Physics, Cornell University — In this study, we fabricated and manipulated single-walled carbon nanotubes (SWNTs) in a liquid medium using microfluidics. The microfluidic system combines manipulative techniques with optical trapping techniques and the scanning photomicroscopy to investigate the motion of suspended single-walled carbon nanotubes in solution. This setup enables us to study the movement of nanotubes by monitoring their photocurrent images and to measure their thermal fluctuations through observing the movement of microbeads that are tightly attached to nanotubes by single-stranded DNA. By analyzing their thermal fluctuations, we are able to obtain the thermal and translational stiffness of nanotubes and then calculate their diameters. We can also manipulate their motions by using an optical trap to pull on microbeads attached to nanotubes.

3:54PM D24.00006 Processing of SWNT Dispersions – Microfluidic Processing vs. Ultrasonication  
TAO LIU, SIDA LUO, CHUCK ZHANG, BEN WANG, High Performance Materials Institute, Florida State University — Ultrasonication is the most commonly used processing technique for dispersing SWNTs in various media. High-power sonication enables the desired dispersibility enhancement and the exfoliation of large SWNT bundles to smaller and even individual tubes. However, one disadvantage for this process is that the SWNT particles can be cut to shorter length. Using a newly developed characterization technique by us for quantifying the structures of SWNTs in a dispersion, we investigated the structural changes of SWNTs due to two different dispersion processing techniques, namely, microfluidic processing and ultrasonication. As a result, the microfluidic processing method shows significantly improved exfoliation efficiency as compared to ultrasonication. Moreover, the length of the exfoliated SWNT particles is maintained upon microfluidic processing, in contrast to the cutting effect caused by the high power sonication. In this presentation, we will discuss in-depth on the processes of SWNT dispersions processed by these two different processing methods.

4:06PM D24.00007 Steric Mode Separation of Nanotubes Using Electric Field, Field-Flow Fractionation  
FREDERICK PHELAN, BARRY BAUER, NIST — A Brownian dynamics simulation is used to study the separation of rodlike particles in Electric Field, Field-Flow Fractionation (EF-FFF), in which in addition to the FFF cross-flow, a uniform AC field acts in the gradient direction. Under these conditions, the electric field acts to align the tubes in the gradient direction in competition with both the shear field and Brownian motion. The simulation results show that as the rods become increasingly aligned, they undergo a transition from normal mode to steric mode separation. By exploiting field conditions in which either metallic or semi-conducting types are preferentially oriented relative to the other, this can be used in the context of nanotube separation as a means for separating tubes by type.
Stokes and antiStokes Raman scattering, from which we infer the mode population of the G-mode phonons. We observe a large nonequilibrium phonon population of the zone-center (G-mode) optical phonons is created by an initial fs laser pulse. A subsequent fs probe pulse generates both 650K. The measurements are performed using a pump-probe Raman scattering scheme with femtosecond (fs) laser pulses [Song et al. PRL 100, 225503 (2008)].

We report on the temperature implications of these models for experiment.

The present work brings a unifying picture to the process of radial compression/deformation of SWNTs, where experimental data are analyzed through a rescaling model yielding a universal-type behavior. Specifically, our AFM measurements show that the quantity

\[ F \propto \frac{1}{r^2} \]

is the SWNT diameter, is a universal function of the compressive strain. Such universality is reproduced analytically in a model where the graphene bending modulus is the only fitting parameter. The application of the same model to the radial Young modulus \( E_r \) leads to a further universal-type behavior that explains the large variations of the SWNTs \( E_r \), reported in the literature. [1] M. S. C. Mazzoni and H. Chacham, Appl. Phys. Lett. 76, 1561 (2000). [2] A. P. M. Barboza et al., Phys. Rev. Lett. 100, 256804 (2008).

Optimal matching of thermal vibrations into carbon nanotubes[1]. K.G.S.H GUNAWARDANA, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma — Carbon nanotubes (CNTs) are promising candidates to improve the thermal conductivity of nano-composites. The main obstacle to these applications is the extremely high thermal boundary (Kapitza) resistance between the CNTs and their matrix. In this work our goal is to maximize the heat flux through the CNT by functionalizing their ends. We develop theoretical continuum models in which we vary the elasticity and density from surrounding medium to the CNT so as to maximize the transmission of thermal vibrations. We calculate the transmission coefficients using a scalar wave equation. Since the transport in CNT is strictly one dimensional, a Landauer formula is used to estimate the heat flux into the CNT. We determine the optimal continuous variation of elasticity and density with position for different geometries. We also investigate how to optimally match the nano-tubes to their matrix using a small number of discrete interfaces. Finally, we discuss the implications of these models for experiment.

This work is supported by the DuPont Co. through a Science & Engineering Grant and NSF grant DMR-0520550.

Temperature dependence of the anharmonic decay of optical phonons in carbon nanotubes and graphite. IOANNIS CHATZAKIS, Columbia University, New York, NY 10027 — The present work was supported in part through the Global COE Program, “Global Center of Excellence for Mechanical Systems Innovation,” by the Ministry of Education, Culture, Sports, and Technology.

Universal response of single-wall carbon nanotubes to radial compression: theory and experiment, HELIO CHACHAM, ANA PAULA M. BARBOZA, BERNARDO R. A. NEVES, Departamento de Física, Universidade Federal de Minas Gerais, Brazil — Since the early 90’s, the electronic and structural properties of single-wall carbon nanotubes (SWNTs) have been thoroughly investigated. Regarding SWNT mechanical properties, most of the attention has been given to their large resistance to axial tension, even though several electromechanical effects have been observed on radially compressed SWNTs, such as the predicted [1], and recently observed [2], metal-insulator transition. The present work brings a unifying picture to the process of radial compression/deformation of SWNTs, where experimental data are analyzed through a rescaling model yielding a universal-type behavior. Specifically, our AFM measurements show that the quantity

\[ F \propto \frac{1}{r^2} \]

is the SWNT diameter, is a universal function of the compressive strain. Such universality is reproduced analytically in a model where the graphene bending modulus is the only fitting parameter. The application of the same model to the radial Young modulus \( E_r \) leads to a further universal-type behavior that explains the large variations of the SWNTs \( E_r \), reported in the literature. [1] M. S. C. Mazzoni and H. Chacham, Appl. Phys. Lett. 76, 1561 (2000). [2] A. P. M. Barboza et al., Phys. Rev. Lett. 100, 256804 (2008).

Carbon Nanomaterials Under Highly Energetic Heavy Ion Irradiation. J.M. CALLAHAN, Michigan State University, B.W. JACOBS, Sandia National Laboratories, C.A., K. MCELROY, M.A. CRIMP, Michigan State University, R.M. RONNINGEN, A.F. ZELLER, National Superconducting Cyclotron Laboratory, H.C. SHAW, NASA Goddard Space Flight Center — The radiation performance of carbon nanomaterials: carbon onions and single-walled carbon nanotubes under highly energetic heavy ion irradiation was investigated, with highly oriented pyrolytic graphite (HOPG) used as the control. Samples were irradiated with a krypton-86 beam at 142 MeV/nucleon, a krypton-78 beam at 140 MeV/nucleon, and a calcium-48 beam at 140 MeV/nucleon and 70 MeV/nucleon at the National Superconducting Cyclotron Laboratory at Michigan State University. Fundamental structural and chemical modifications were investigated using Micro Raman spectroscopy and high-resolution transmission electron microscopy (HRTEM). Results indicated that the radiation resiliency of the single-walled carbon nanotubes exceeded that of highly oriented pyrolytic graphite, while the carbon onions showed structural modifications of the outer onion layers in the form of facetting and onion fusion.


Synthesis, characterization and thermal stability of CVD-grown graphene nanoribbons. JESSICA CAMPOS-DELGADO, Advanced Materials Department, IPICYT, Mexico, Y.A. KIM, ENDO MORINOBO, Shinhu University, Japan, KATSUHI KANeko, Chiba University, Japan, HUMBERTO TERRONES, IPICYT, Mexico, MILRED S. DRESSELHAUS, ECCS, MIT, USA, MAURICIO CIRO TERRONES, IPICYT, Mexico — A route to produce large amounts of nanometer scale graphene ribbons is presented. The process involves the thermal decomposition of ethanol-ferrocene and minute concentrations of thiophene solutions. The material consists of stacked graphene sheets with dimensions of several microns in length, 100-500 nm in width and 10-20 nm in thickness. The morphology and structure of such material have been studied by SEM, HRTEM, Raman spectroscopy, XRD, XPS, TGA. In order to investigate the thermal stability of the pristine material, the as-prepared ribbons were annealed at various temperatures in the range 1000 °C to 2800 °C. The annealing treatments induced interesting structure changes in the samples, such as defect annihilation and loop formation at the edges, confirmed by HRTEM. A Raman spectroscopy study with many laser energies, enabled us to observe the overall behavior of the main Raman features (D, G, D', G', D+G bands). These phenomena will be discussed in detail.
2:42PM D25.00002 Nitrogen-induced structures in epitaxial graphene on 6H-SiC(0001)

GUOFENG SUN, SUNG-HYON RHM, University of Wisconsin-Milwaukee, YUN QI, MICHAEL WEINERT, LIAN LI, University of Wisconsin-Milwaukee — Nitrogen-induced structures on epitaxial graphene grown on 6H-SiC(0001) are studied by scanning tunneling microscopy (STM) and first-principles calculations. Several defect structures produced by nitrogen incorporation are observed by STM. Calculations of the energetics of nitrogen substitution at various sites neighboring a carbon vacancy indicate that nitrogen prefers to be at the site nearest to the vacancy, consistent with the STM observations.

3:30PM D25.00004 Kelvin Probe Microscopy of Single- and Multi-layer Graphene on SiO$_2$

ALEXANDRA CURTIN, University of Maryland, THERESA SWANSON, Westminster College, MICHAEL S. FUHRER, Materials Research Science and Engineering Center and Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — Kelvin probe microscopy (KPM) was carried out on mechanically exfoliated graphene samples on SiO$_2$ in conjunction with standard atomic force microscopy. Potential differences between the SiO$_2$ substrate and graphene flakes were large relative to the average fluctuations over the surface of the graphene. KPM shows a consistent surface potential variation between monolayer, bilayer, and multi-layer graphene, and over folded pleats occasionally found in graphene. The source of these surface potential differences will be discussed.

4:06PM D25.00007 Planar tunneling spectroscopy of graphite

RICHARD JONES, WAN KYU PARK, SAM JOHNSON, XIN LU, NADYA MASON, LAURA GREENE, University of Illinois at Urbana-Champaign — The electronic properties of graphite/graphene have become an intriguing area of research in recent years. Probing their electronic density of states (DOS) is of fundamental importance. For this purpose, we choose to do tunneling spectroscopy based on planar junctions. We prepare planar tunnel junctions on graphite using superconducting and normal metal counter-electrodes. An AlO$_3$ tunnel barrier is deposited onto a cleaved surface of HOPG using atomic layer deposition, reactive sputtering, thermal oxidation, or plasma oxidation. Differential conductance spectra are taken as a function of temperature down to 4.2K. In general, conductance increases with bias-voltage, which is qualitatively consistent with the predicted DOS in graphite. However, variances in the detailed structures are observed, including a zero-bias conductance dip and multiple peak and hump structures. We will also discuss different growth techniques we propose to yield reproducible junction characteristics.

4:42PM D25.00003 Large area, Few Layer Graphene Films on Insulating Substrates

JING KONG, Massachusetts Institute of Technology — Graphene has exceptional electronic, thermal and mechanical properties. For the realization of graphene-related applications, it is necessary to develop reliable and low cost fabrication methods of graphene-based structures, ideally on any substrates. In this talk I will present our method of fabricating large area (~cm$^2$) films of single- to few-layer graphene and transferring the films to arbitrary substrates. The graphene films are synthesized by ambient pressure Chemical Vapor Deposition, consist of regions of 1 to ~10 graphene layers and have an average thickness of 2-3 nm. Despite their ultra-thin nature, the films thus produced are continuous over the entire area. Regions of single- or bi-layer graphene with lateral sizes of up to 25 $\mu$m were observed. High Resolution Transmission Electron Microscopy (HRTEM) and electron diffraction revealed that they are crystalline over the entire area and their Raman features were compared to those of graphene derived from mechanical exfoliation of Highly Oriented Pyrolytic Graphite (HOPG). Transistor devices made from these graphene show similar characteristics to ones made from graphitized SiC. Scanning tunneling microscopy imaging reveals interesting Moré patterns and helpful insights for the growth of the graphene films on the Ni substrate. The method presented in this work can potentially be scaled to industrial production of graphene films, for applications such as ultra-thin conductive and transparent electrodes, or devices and interconnect for integrated circuits.
4:42PM D25.00010 Electrical Transport in Graphene Hybrid Structures, FENG MIAO, WENZHONG BAO, HANG ZHANG, CHUN NING LAU, Department of Physics and Astronomy, University of California, Riverside, CA 92521 — Graphene, monolayer carbon atoms with honeycomb lattice, has intrigued condensed matter physics field for its unique electrical properties since its first discovery in 2004. The graphene hybrid structures that consist of both single and bi-layers were also experimentally studied recently for its novel properties. We will present our experimental study on the electron transport in graphene hybrid structures and the latest experimental data will be discussed in terms of various theoretic models.

4:54PM D25.00011 Dependence of the Low Energy Electronic Structure of Multi-layer Graphene on Stacking Order Probed by Infrared Absorption, MATTHEW SFIEIR, KIN FAI MAK, JAMES MISEWICH, TONY HEINZ, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 COLLABORATION, BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973 COLLABORATION — Optical conductivity spectra of multi-layer graphene samples were determined for photon energies in the range of 0.2 – 1.0 eV. The measurements were performed using synchrotron radiation on well-characterized exfoliated graphene samples on a transparent substrate. We observed distinct optical conductivity spectra for different samples having precisely the same number of layers. In particular, two well-defined types of spectra were obtained in measurements of more than a dozen of four-layer samples. This result can be understood by considering the existence of two stable configurations of four-layer graphene, namely, the ABAB Bernal stacking and the ABCA rhombohedral stacking. The observed absorption features were reproduced by explicit calculations, within a tight-binding model of the optical conductivity for the two stacking sequences. We have thus shown the possibility of identifying these different crystallographic structures optically. Further, the significant difference found in the low-energy electronic structure suggests that the charge transport behavior of multilayer graphene may also depend on stacking order.

5:06PM D25.00012 AFM study of the ridge-like network on epitaxial few-layer graphene grown on 4H-SiC [0001], GYAN PRAKASH, Dept. of Physics and Birck Nanotechnology center, Purdue U., W. Lafayette 47907, MICHAEL CAPANO, MICHAEL BOLEN, School of Electrical Eng. and Birck Nanotechnology center, Purdue U., W. Lafayette 47907, DMITRY ZEMLYANOV, Birck Nanotechnology center, Purdue U., W. Lafayette 47907, RONALD REIFENBERGER, Dept. of Physics and Birck Nanotechnology center, Purdue U., W. Lafayette 47907 — Few-layer graphene (FLG) is produced when SiC is heated to temperatures T>1475°C under vacuum conditions. The FLG grown on SiC exhibits a 2D mesh of interconnected ridges that extends over many square microns. Smooth regions of FLG are surrounded by the 2D ridges, forming a tile-like surface morphology. The origin of the network is attributed to the compressive stress generated by cooling. For FLG growth at moderately higher temperatures, the thickness of the FLG increases. Under these conditions, AFM studies reveal the emergence of a few well-defined folds that relax the surface stress. In contrast to the previous ridge-like network, the folds appear at only a few locations and have a greater height than the ridges. This AFM study provides insights on how to improve the quality of FLG material grown at elevated temperatures on SiC substrates.

5:18PM D25.00013 Moiré Patterns: Fingerprints of Few-Layer Epitaxial Graphene Growth on 4H-SiC(0001), LAURA BIEDERMANN, Dept. of Physics and Birck Nanotechnology Center, Purdue University, MICHAEL BOLEN, MICHAEL CAPANO, School of Electrical Engineering and Birck Nanotechnology Center, Purdue University, DMITRY ZEMLYANOV, Birck Nanotechnology Center, Purdue University, RONALD REIFENBERGER, Dept. of Physics and Birck Nanotechnology Center, Purdue University — Few-layer epitaxial graphene (FLG) was grown on heating [0001] silicon carbide to high temperatures (1350–1600°C) in vacuum. A continuous graphene surface layer was formed at temperatures of 1475°C and greater. X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM) were used to characterize the quality, thickness, and topography of the FLG. STM studies revealed a wide variety of different nanometer-scale features that include rough graphene, 1D superlattices, grain boundaries, and Moiré 2D superlattices. Detailed studies of the Moiré superlattices showed enhanced conductivity due to density of states effects. These Moiré superlattices also provided insights into the growth mechanisms of FLG on the carbon-face of SiC. L. Biedermann et al., “Insights into Few-Layer Epitaxial Graphene Growth on 4H-SiC(0001) Substrates from STM Studies,” Phys. Rev. B (submitted).

Monday, March 16, 2009 2:30PM - 5:30PM — Session D26 DMP DCOMP: Focus Session: Computational Nanoscience III: Defects, Doping, and Structure 328

2:30PM D26.00001 Intrinsic magnetism in nonmagnetic nanostructures: Role of localized states and quantum confinement1, PEIHONG ZHANG, University at Buffalo, SUNY — Manipulation of carrier spins in semiconductors for spintronics applications has received much attention recently driven by the promise of new or improved functionalities. This has stimulated extensive research in the area of magnetic semiconductors. Magnetism is traditionally recognized as arising from unpaired electrons in 3d and 4f materials. However, there has been increasing evidence that localized defect states (and/or surface/edge states) in sp materials, especially in some nanostructures, may form local moments and exhibit collective magnetism. In a recent paper [PRL100, 117204 (2008)], we proposed that the duality (i.e., localized vs extended nature) of defect states in wide-gap nitrides and oxides may promote collective magnetism in these materials without magnetic ions. We have recently extended this study to include unexpected magnetism observed in GaN and ZnO nanowires and other artificial quantum structures. Particular attention will be paid to the role of localized states and quantum confinement in promoting unconventional magnetism in these systems.

3:06PM D26.00002 Defect induced magnetism in semiconductor nanostructures1, HYUNWOOK KWAK, University of Minnesota, TZU-LIANG CHAN, JAMES CHELIKOWSKY, University of Texas — It has been proposed that magnetic semiconductors can be designed by using non-magnetic defects, e.g., through the introduction of an extrinsic impurity atom that does not exhibit magnetism by itself (Phys. Rev. Lett. 99, 127201). In order to address such proposals, we have employed a real-space pseudopotential method based on the generalized gradient approximation to determine the magnetic properties of boron and aluminum doped silicon nanocrystals and nanowires. We will discuss theoretical evidence for defect induced magnetism as a function of the nanostructure size. We suggest that defect induced magnetism can be strongly enhanced by quantum confinement.

1This work was supported in part by National Science Foundation Grant No. CBET-0844720 and by the UB 2020 Interdisciplinary Research Development Fund (IRDF).

2This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.
3:18PM D26.00003 Ferromagnetism driven by extended defects in nanostructured ZnO

ALINE L. SCHOENHALZ, JEVERTON T. ARANTES, ADALBERTO FAZZIO, GUSTÃO M. DALPIAN, Universidade Federal do ABC — Spintronics has a particular interest in diluted magnetic semiconductors because these materials present both semiconducting and magnetic properties at the same time. ZnO-based materials and nanostructures have potential applications in this area because they can present room-temperature ferromagnetism when doped with transition metals and, in some cases, spin polarization can be observed even without magnetic impurities. Following recent experimental results reporting this (Nano Lett. 6, 1489 (2007) )), we have analyzed several ZnO nanocrystals, with diameters varying from 0.9 to 1.78 nm. Using DFT, we observed that a large amount of surface reconstructions appear in the non-passivated nanocrystals. Depending on the reconstruction, spin polarization without magnetic impurities can be observed at the surface region, what can lead to long-range spin interactions. Thus, we propose that the referred experimental results for nanostructured ZnO can be originated by extended defects such as surfaces. This can also explain the same magnetic behavior presented by non-doped thin films and other ZnO nanostructures.

3:20PM D26.00004 Self-doping in Boron Nanostructures

HUI TANG, SOHRAB ISMAIL-BEI, Department of Applied Physics, Yale University — Boron nanotubes with large radii (R > 10 Å) are predicted to be metallic with large densities of states at their Fermi energies, which may provide excellent conducting systems for one-dimensional electronics. In previous work [1], we have shown a class of stable boron sheets, composed of mixtures of triangular and hexagonal motifs, that are likely to be the precursors of boron nanotubes. These sheets are stabilized by a balance of 2-center and 3-center bonding. Here, using density functional theory and Maximally Localized Wannier Functions, we show that adding a boron atom to a boron sheet is equivalent to doping the boron sheet with all three valence electrons of the added atom. Based on this self-doping picture, we propose a simple counting scheme to construct stable boron nanostructures, e.g. from corresponding carbon wanniersons. We also apply this knowledge to study Mg-doped boron sheets and discuss the possible stable structures of MgB2 nanotubes.

3:22PM D26.00005 Computational Studies of Nanostructures of Boron

P. TANDY, M. YU, C. LEAHY, University of Louisville, W.Q. TIAN, Jilin University, S.Y. WU, C.S. JAYANTHI, University of Louisville, U. OF LOUISVILLE/JILIN U. — The goal of this work is to develop a reliable semi-empirical Hamiltonian for boron that may be used to predict nanostructures of boron. It is well known that bonding in boron is complicated as it may form three-center, two-electron bonds. The semi-empirical Hamiltonian used here was recently developed by Leahy et al. in the framework of linear combination of atomic orbitals [1]. The salient feature of this Hamiltonian is that it treats environment dependency and charge redistributions on equal footing. It will be shown that such a parameterized Hamiltonian can predict the B80 cage structure with C2V symmetry as found in a recent first-principles study [2]. Having validated our semi-empirical Hamiltonian for boron with small boron clusters and the B80 cage, we have performed a systematic study of other boron nanostructures: (i) larger cage structures (e.g., B215), (ii) boron clusters cut from the bulk alpha boron, and (iii) boron sheets (triangular sheets with and without holes). We will discuss the ground state structures of these boron nanostructures as well as the energetics and HOMO-LUMO gaps of different families of boron clusters as a function their diameters.

3:42PM D26.00005 Computational Studies of Nanostructures of Boron

P. TANDY, M. YU, C. LEAHY, University of Louisville, W.Q. TIAN, Jilin University, S.Y. WU, C.S. JAYANTHI, University of Louisville, U. OF LOUISVILLE/JILIN U. — The goal of this work is to develop a reliable semi-empirical Hamiltonian for boron that may be used to predict nanostructures of boron. It is well known that bonding in boron is complicated as it may form three-center, two-electron bonds. The semi-empirical Hamiltonian used here was recently developed by Leahy et al. in the framework of linear combination of atomic orbitals [1]. The salient feature of this Hamiltonian is that it treats environment dependency and charge redistributions on equal footing. It will be shown that such a parameterized Hamiltonian can predict the B80 cage structure with C2V symmetry as found in a recent first-principles study [2]. Having validated our semi-empirical Hamiltonian for boron with small boron clusters and the B80 cage, we have performed a systematic study of other boron nanostructures: (i) larger cage structures (e.g., B215), (ii) boron clusters cut from the bulk alpha boron, and (iii) boron sheets (triangular sheets with and without holes). We will discuss the ground state structures of these boron nanostructures as well as the energetics and HOMO-LUMO gaps of different families of boron clusters as a function their diameters.

4:06PM D26.00007 Graph-based global optimization of fully-coordinated cluster geometries

EDWIN FLITKEEMA, Aberystwyth University, UK, STEFÁN BROMLEY, Universitat de Barcelona, Spain — To study systems with substitutional disorder researchers commonly use effective Hamiltonians known as cluster expansions. In a cluster expansion the phase space of a system is coarse-grained over a fixed set of crystal sites and the energy is expressed as a linear combination of interactions between these sites. The coefficients of the linear expansion are typically fit to training data generated using ab-initio methods. Low-symmetry systems such as nanoparticles require the determination of a large number of distinct coefficients. A large amount of training data must be generated for such problems, and the cost of calculating the energy of each training structure is high due to the low symmetry of the system. For these reasons it has been impractical to use the cluster expansion to study low-symmetry materials with the same level of accuracy as bulk materials. We address this problem by demonstrating new methods that significantly reduce the prediction error of a cluster expansion for a given training set size. Our approach makes it possible to study atomic ordering in nanoparticles at a fraction of the current computational cost.

4:18PM D26.00008 Nanostructure determination from the atomic pair distribution function

LUKE GRANLUND, Michigan State University, PAVOL JUHAS, Columbia University, SAURAB GUJARATHI, PHIL DUXBURY, Michigan State University, SIMON BILLINGLE, Columbia University — Many materials at the nanoscale cannot benefit from crystallographic analysis and are unsuitable for refinement techniques that require an initial guess at the structure. One approach to overcoming these difficulties is the Liga algorithm, which generates structures relying solely on distances extracted from the atomic pair distribution function [1,2]. This method is shown to successfully reconstruct the buckyball from experimental data. Recent extensions to multi-component and periodic systems have also allowed reconstruction of common crystals from experimental data. The ability to handle both periodic and nonperiodic cases may make the algorithm a useful tool in the study of local structure deviations in nanocrystals in addition to noncrystalline nanomaterials. [1] P. Juhas, D. M. Cherba, P. M. Duxbury, W. F. Punch, S. J. L. Billinge. Ab initio determination of solid-state nanostructure. Nature, 440, 655-658 (2006). [2] P. Juhas, L. Granlund, P. M. Duxbury, W. F. Punch, S. J. L. Billinge. The Liga algorithm for ab initio determination of nanostructure. Acta Cryst., A64, 631-640 (2008).
4:30PM D26.00009 The role of confinement on the diffusion barriers in semiconductor nanocrystals¹, Tzu-Liang Chan, Alexey Zayak, University of Texas at Austin, Gustavo Dalpian, Universidade Federal do ABC, James Chelikowsky, University of Texas at Austin — We find that quantum size effects not only play an important role in the electronic properties of defects in semiconductor nanocrystals, but also strongly affect the incorporation of defect atoms into the nanocrystals. In particular, using ab initio methods based on density functional theory, we predict that Mn defects will be energetically expelled to the surface of CdSe and ZnSe nanocrystals, and that the diffusion barriers of a Mn interstitial defect in a CdSe nanocrystal will be significantly lower than that in the bulk. This can be ascribed to the large surface to volume ratio of nanocrystals, which can effectively release the strain during diffusion. By calculating the vibrational spectrum of the CdSe nanocrystal, we estimated the diffusion rate within the nanocrystal. Our results suggest that energetics can play a role in the self purification of small CdSe and ZnSe nanocrystals, as diffusion of the defect atom can readily occur inside such small nanocrystals.¹

¹This work was supported in part by National Science Foundation under DMR-0551195 and the U. S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760. GMD thanks financial support from FAPESP and CNPq.

4:42PM D26.00010 Accelerated Kinetic Monte Carlo Simulations of Vacancy-Mediated Arsenic Diffusion and Clustering in Silicon, Brian Puchala, University of Michigan, Michael Falk, Johns Hopkins University, Krishna Garikipati, University of Michigan — During semiconductor device fabrication, ion implantation of dopants creates large populations of defects, vacancies and interstitials, which mediate dopant diffusion. Experiments have shown large changes in dopant diffusivity in silicon as a function of annealing time and dopant concentration in the proximity of their critical concentrations. Kinetic Monte Carlo (KMC) simulations of vacancy-mediated arsenic diffusion in silicon to investigate the effect of dopant concentration, distribution and clustering on diffusivity. In order to follow the diffusion and breakup of clusters, on the order of minutes, our KMC simulations are accelerated using absorbing Markov chain analysis on states intelligently chosen on-the-fly to fill trapping basins in the local energy landscape. At lower dopant concentrations, we calculate the diffusivity and breakup rates of different cluster types and a mean field approach can be used to describe the overall cluster population evolution and dopant diffusivity. Above a critical concentration this mean field description fails as dopants become close enough to form a percolating structure throughout the material. At all concentrations, diffusivity decreases significantly over time as larger, less mobile clusters form.

4:54PM D26.00011 First Principles Study of the Effect of Lattice Strain on Diffusion Barriers¹, Handan Yildirim, Talat S. Rahman, University of Central Florida — To understand the three times larger values of the Erlich Schoewebel barriers for Ag on Cu(100) as compared to that for Cu on Ag(100), as obtained from our density functional theory calculations, we performed the diffusion of Ag adatom on Ag(100) and Cu adatom on Cu(100) under uniform lattice strain of 0-5%. We find the origin of the differences in the energetics to be the combination of Cu-Ag electronic coupling, relative atomic sizes and adsorbate-substrate lattice mismatch. The diffusion barriers on the ideal surfaces are found to decrease with increasing compressive strain and to increase with increasing tensile strain and almost a linear function of strain up to 5%. We show that this trend is universal and transferable to other materials. We will discuss the consequences of the modifications in the height of the ES barriers on growth modes.

¹This work was supported by the National Science Foundation under DMR-0551195 and the U.S. DOE under DE-FG02-06ER46286 and DE-FG02-06ER15760.

5:06PM D26.00012 Quantum confinement in P-doped Si[110] nanowires¹, Jiaxin Han, Tzu-Liang Chan, James Chelikowsky, University of Texas at Austin — Recently, doped Si nanowires have been synthesized and demonstrated experimentally that they can be used as interconnects in electronic circuits or building blocks for semiconductor nanodevices. In order to understand how doping operates at the nanoscale, we used a real-space first-principles pseudopotential method to study P-doped Si[110] nanowires. We examined the size dependence of the electronic binding energy for the P donor level. We found the donor electron to be more strongly bound to the P atom with decreasing nanowire diameter owing to quantum confinement. We also examined the energetically favorable position of the P atom in Si nanowires. For nanowires with diameter less than 1 nm, the P atom is expelled to the surface owing to the stress induced by the defect, which suggests that doping will be difficult for small-diameter Si nanowires. In addition, we calculated the core-level binding energy shift as the P atom moves from the surface towards the center of the nanowire. We will compare our results with experimental measurements.

¹This work was supported by the National Science Foundation under DMR-0551195 and the U.S. DOE under DE-FG02-06ER46286 and DE-FG02-06ER15760.

5:18PM D26.00013 Effect of structure, surface passivation, and doping on the electronic and optical properties of GaAs nanowires: A first principles study,¹ S. V. Khare, Dept. of Physics, V. Gade, Dept. of EECS, University of Toledo, N. Shi, R. Ramprasad, Dept. of Chemical, Materials, and Biomolecular Engineering, Univ. of Michigan — We investigate the structural, energetic, electronic, and optical properties of hydrogen-passivated doped and undoped gallium arsenide nanowires along [001], [110], and [111] directions with diameter d ≤ 3 nm, using ab initio methods. A critical diameter d̃ ≈ 2 nm is found above which all wires have faceted cross sections determined by the symmetry of their axis. The wires possess several electronic properties relevant for sensing and other nanoelectronic applications: (i) Quantum confinement has a substantial effect on the electronic band structure and hence the band gap (Eg), which increases with decreasing diameter. (ii) Unlike Si or Ge wires, GaAs wires oriented along all axes are found to have a direct Eg. (iii) The electronic band structure shows a significant response to changes in surface passivation with hydrogen. (iv) Doping of wires with n and p type atoms produces a response in the band structure similar to that in a doped bulk crystal. (v) However, the dielectric function shows differences in absorption peaks with p type versus n type doping.

¹We thank WPAFB, PVIC, and NSF-DMR for funding this work.

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D27 GIMS: Advances in Instrumentation and Measurement I 329

2:30PM D27.00001 Mechanical properties of silicon nanowires studied by polarization-enhanced fiber-optic interferometry¹, John Nichol, University of Illinois at Urbana-Champaign, Eric Hemesath, Lincoln Lauhon, Northwestern University, Raffi Budakian, University of Illinois at Urbana-Champaign — Silicon nanowires have recently attracted attention as promising force sensors due to their inherent low dissipation and high frequency. One of the principal challenges to the use of nanowires as scanning probe force sensors is displacement detection. By exploiting the polarization anisotropy in light scattering from single nanowires, we have used fiber-optic interferometry to detect the displacement of individual silicon nanowires. We achieve a displacement sensitivity of 0.5 pm/vHz for 15 µW of light incident on the nanowire. The nanowires studied have ultralow mechanical dissipation in the range of 2×10⁻¹⁵-2×10⁻¹⁴ kg/s. We also discuss the effects of hydrogen surface passivation on mechanical dissipation. Further progress toward the use of nanowires as scanning probe force sensors is discussed.

¹This work was supported by the ARO (MURI grant W911NF-05-0414) at the University of Illinois and by the NSF (NIRT program) at Northwestern University.
I. Electromagnetic fluctuations cause the power law suppression at low voltages, transport through a quantum dot in the Coulomb blockade regime. We obtain the analytic expression for the elastic cotunneling current which shows that the magnetic fluctuations.


By attaching these single spins to the tip of a scanning probe, we were able to perform sensitive scanning probe magnetometry at nanoscale.

II. Precise measurements of individual colloidal spheres’ dimensions and optical properties, while simultaneously tracking their three dimensional motions with highly resolved in-line holographic video microscopy, can be interpreted with Lorenz-Mie theory to obtain exceptionally high spatial resolution. We assert that additional analysis of the secondary electrons will also exhibit a comparable resolution.

III. Synchrotron-based angle-resolved photoemission spectroscopy has proven to be a powerful tool in the elucidation of electronic structure of solids. The technique is now being applied to a wide variety of materials, and the macroscopic sampling area has become a limitation. For example, cleaving may expose different crystal planes, and the area covered by the incident photon beam may then consist of a collection of small domains with different photoemission spectra. The result is an average which obscures the true nature of the material. For this reason a beamline with a small focus has been proposed to be used with an angle-resolved photoemission endstation at the Synchrotron Radiation Center in Stoughton, WI. Reflective optics would be used to produce a microfocus at the sample of the light from an undulator beamline, providing submicron spatial resolution, while electron emission angles and energies are measured using an imaging electron energy analyser. The microfocusing optics and possible applications will be discussed.

IV. Second harmonic technique to be used eventually to probe the thermal conductivity of LSCO with superconductivity suppressed by high magnetic fields. The technique is suitable for the high-noise environment of pulsed magnets. Unlike the $3\omega$ technique, a heater and a thermometer are mounted separately. Therefore, the $2\omega$ signal is the dominant signal in the thermometer output. The frequencies are chosen so that the thermal penetration depth is smaller than the sample thickness. The thermometer response time and thermal impedance associated with material interfaces are carefully tested and compared to calculation. The calculations are based on exact solutions of the full bulk heat transport equations and produce results different from the lumped-constant approximations often used in ac calorimetry. Work performed under the auspices of the National High Magnetic Field Laboratory.

V. The technique is suitable for the high-noise environment of pulsed magnets. Unlike the $3\omega$ technique, a heater and a thermometer are mounted separately. Therefore, the $2\omega$ signal is the dominant signal in the thermometer output. The frequencies are chosen so that the thermal penetration depth is smaller than the sample thickness. The thermometer response time and thermal impedance associated with material interfaces are carefully tested and compared to calculation. The calculations are based on exact solutions of the full bulk heat transport equations and produce results different from the lumped-constant approximations often used in ac calorimetry. Work performed under the auspices of the National High Magnetic Field Laboratory.

2:42PM D27.00002 Zero Flux Anomaly in Mesoscopic Normal Metals , JULIE BERT, HENDRIK BLUHM

2:54PM D27.00003 Second Harmonic Technique for Thermal Conductivity Measurement in a Pulsed Magnetic Field , YOKO SUZUKI, JONATHAN B. BETTS, ALBERT MIGLIORI

3:06PM D27.00004 Nanoscale imaging magnetometry with single spins in diamond, GOPALKRISHNAN BALASUBRAMANIAN, JULIA TISLER, ROMAN ROLESOV, FEDOR JELEZKO, JOERG WRACHTRUP

3:18PM D27.00005 Elastic cotunneling through a quantum dot in the presence of electromagnetic fluctuations, VLADIMIR BUBANJA

3:30PM D27.00006 Grapenated Infrared Screens: A New Platform for Bio-Detection, AMRITA BANERJEE, DIETER MOELLER, HAIM GREBEL

3:42PM D27.00007 Development of a Microfocus Beamline for Angle-Resolved Photoelectron Spectroscopy, T. MILLER, Univ. of Illinois at Urbana-Champaign, M. BISSEN, Univ. of Wisconsin Synchrotron Radiation Center, T.-C. CHIANG, Univ. of Illinois at Urbana-Champaign — Synchrotron-based angle-resolved photoemission spectroscopy has proven to be a powerful tool in the elucidation of electronic structure of solids. The technique is now being applied to a wide variety of materials, and the macroscopic sampling area has become a limitation. For example, cleaving may expose different crystal planes, and the area covered by the incident photon beam may then consist of a collection of small domains with different photoemission spectra. The result is an average which obscures the true nature of the material. For this reason a beamline with a small focus has been proposed to be used with an angle-resolved photoemission endstation at the Synchrotron Radiation Center in Stoughton, WI. Reflective optics would be used to produce a microfocus at the sample of the light from an undulator beamline, providing submicron spatial resolution, while electron emission angles and energies are measured using an imaging electron energy analyser. The microfocusing optics and possible applications will be discussed.

3:54PM D27.00008 Near field emission scanning electron microscopy, TARYL KIRK, LORENZO DE PIETRO, OLIVIER SCHOLDER, THOMAS BAehler, URS RAMSPERGER, Danilo Pescia, Swiss Federal Institute of Technology Zurich (ETHZ) — We present a simple “near field emission scanning electron microscope” (NFESEM) capable of imaging conducting surfaces with high spatial resolution. In this instrument electrons are excited from the sample surface after undergoing interactions with a low-voltage (< 60V) primary beam of electrons emitted from a Tungsten tip positioned tens of nanometers above the sample. Topographic images, determined from the intensity variations of secondary and backscattered electrons, yield a vertical resolution on an atomic scale and a lateral resolution of less than two nanometers. We report on the first topographic electron intensity images of terraces and mono-atomic steps on a single crystal substrate, not yet attained with a remote electron gun in conventional scanning electron microscopy. The topographic contrast of the extracted electrons and the field emission (FE) current are indistinguishable, in agreement with theoretical models of optimal spatial resolution. We assert that additional analysis of the secondary electrons will also exhibit a comparable resolution.

4:06PM D27.00009 Particle Characterization using Holographic video Microscopy, FOO CHIONG CHEONG, DAVID GRIER, New York University — In-line holographic video microscopy can be interpreted with Lorenz-Mie theory to obtain exceptionally precise measurements of individual colloidal spheres’ dimensions and optical properties, while simultaneously tracking their three dimensional motions with nanometer-scale spatial resolution at video rates. This method works over the entire range of particle sizes and compositions for which Mie scattering theory applies. Unlike other light scattering techniques for measuring particle size or refractive index, holographic particle analysis can be applied directly to individual particles.
4:18PM D27.00010 Three-dimensional position determination of nanoparticles using a two-photon microscope. JAMES GERMANN, LLOYD DAVIS, BRIAN CANFIELD, ALEXANDER TEREKHOV, University of Tennessee Space Institute - Center for Laser Applications — We are developing a means to extend the two-photon microscope to enable three-dimensional sub-diffraction measurement of the position and trajectory of a single nanoparticle as it traverses the probe volume. By use of a Ti-Sapphire laser and a double-Mach-Zehnder interferometer configuration, four laser beams with temporally interleaved pulses are created. These are tightly focused by a 1.2-NA water-immersion microscope objective to four overlapping volumes centered at slightly offset points arranged in a tetrahedron. Fluorescence from the four-focus probe volume is then collected onto a single-photon avalanche diode and the photon time stamps are recorded. Time-resolved photon detection with maximum-likelihood analysis is thereby used to determine the position of the nanoparticle from the relative intensities of fluorescence from each of the four foci. We present measurements of the profile of the four-focus configuration and results from calibration experiments obtained by translating a single gold nanodot or a fluorescent nanobead through the probe volume. Application of the position determination to single-particle trapping is also briefly discussed.

4:30PM D27.00011 Capabilities of high-sensitivity spectral fluorescence-lifetime imaging for resolving spectroscopically overlapping species. JUSTIN CRAWFORD, University of Tennessee Space Institute - Center for Laser Applications, LLOYD DAVIS, BRIAN CANFIELD, University of Tennessee Space Institute — The ability to separate the contributions from spectroscopically overlapping fluorophores has enabled significant breakthroughs in cellular imaging. However, commercial microscopes for this purpose generally use analog light detection with least-squares curve-fitting analysis. Improvements in sensitivity are possible and will lead to new applications. To this end, we have constructed a microscope with a high-throughput Brewster-prism spectrometer and four high-quantum efficiency single-photon detectors, coupled with time-correlated single photon counting electronics to provide added temporal resolution. We have demonstrated the use of maximum-likelihood (ML) methods for analyzing small numbers of photons to find the contributions from fluorescent species with differences in excitation and emission spectra. However, it is difficult to resolve fluorophores with different temporal decay profiles because the single-photon counting modules exhibit a count-rate-dependent time-walk. We discuss extension of the ML-analysis to account for a varying time-walk and results from Monte Carlo simulations to ascertain the minimum number of photons needed to reliably resolve specific fluorophores.

4:42PM D27.00012 Development of a low-cost small-sized scanning transmission ion microscope of moderate resolution with educational and other potential applications. ARTHUR PALLONE, Murray State University — Scanning transmission ion microscopy (STIM) has applications in many fields of study such as materials and device engineering, biological and geological sciences, and the arts. Since STIM is practiced at ion beam facilities, many persons outside of the ion beam community who could benefit from STIM are unaware of its potential. In an effort to better educate the public about STIM, an inexpensive portable demonstration unit suitable for interactive classroom use and public outreach events is under development. The required parts are readily available, mostly at local electronics and office supply stores. Progress toward completion of the demonstration unit and future efforts to modify the unit to support thin film research will be discussed. Activities that demonstrate the three modes of STIM will also be presented.

4:54PM D27.00013 A two dimensional piezoelectric micro-positioner1. K.-W. NG, JOHN NICHOLS, J. W. BRILL, University of Kentucky — A scanning probe microscope can provide very high resolution imaging, but only within a small scanning area. There is a high demand for compact long range positioners, so that distant locations on the same sample can be imaged and studied. We will present information on the design and operation of a piezoelectric driven two-dimensional micropositioner that can provide long range motion in the x- and z-directions. The z-direction motion can be used for coarse approach, while the x-direction motion can be used to scan along the sample surface. The device is build as one single unit, so it is extremely compact and rigid, and can provide a high resonance frequency platform for high performance scanning probe microscopy.

5:06PM D27.00014 High Speed Scanning Property Mapping (>1 frame per second)1. BRYAN HUEY, NICHOLAS POLOMOFF, ATIF RAKIN, VINCENT PALUMBO, University of Connecticut, Institute of Materials Science — Atomic Force Microscopy is coupled with concepts of acoustics to achieve nanoscale property contrast at line scanning rates approaching several kHz. This allows novel measurements of surface dynamics, efficient large area imaging, and high throughput experiments with SPM. Examples for mechanical contrast on block copolymers, semiconductors, and eutectic alloys are included, as well as high speed electric and magnetic field imaging. Coupled electromechanical contrast (piezoelectric) is also employed with PZT thin films to uniquely monitor ferroelectric domain dynamics.

5:18PM D27.00015 Method for Detecting Position and Orientation of Convex Objects in 3D Scans, ALEXANDER JAOSHVILI, PAUL CHAIKN, NYU — We have developed an algorithm for detecting the center positions and orientations of monodisperse objects which pack a container from the data collected in a 3 dimensional scan such as obtained by MRI. The algorithm is applied to a variety of geometrical convex shapes including, ellipsoids, cubes and tetrahedrons. From the positions and orientations we are able to reconstruct the number and type of interparticle contacts and constraints and thus to test Maxwell’s isostatic conjecture in the case of “random close packing.” We also obtain translational and orientational correlation functions.

Monday, March 16, 2009 2:30PM - 5:18PM_
Session D28 DMP FLAP: Focus Session: Thermolectric Materials: Oxides and Complex Crystals 330

2:30PM D28.00001 Thermoelectricity in oxides and weakly coupled single molecules. SUBROTO MUKERJEE, University of California, Berkeley — Complex oxides have emerged as promising candidate materials for thermolectric and energy applications. The study of charge and heat transport in these systems is also very interesting and important from the point of view of fundamental physics. We show that oxides in the narrow-bandwidth limit have high values of the thermopower and power factor and also violate the Wiedemann-Franz law yielding high values of the electronic part of the figure of merit. These theoretical results agree with the data on Na$_x$CoO$_2$. We argue that in another oxide Sr$_{1-x}$La$_x$TiO$_{3−δ}$, a large effective mass (small bandwidth) band appears due to oxygen vacancies, which can be exploited for thermolectric applications and comment on recent experiments. Finally, we show that there are commonalities in the thermoelectric behavior of narrow bandwidth oxides and weakly coupled single molecules. The latter systems also offer promise as thermolectric materials due to the possibility of large values of thermopower and we comment on the limiting effect of phonons on their figures of merit.
3:06PM D28.00002 Magneto-Spectroscopic Measurements of Ca$_3$Co$_2$O$_9$ Thin Films and Single Crystals\textsuperscript{1} JIUFENG TU, DIMITAR DIMITROV. The City College of New York, WEIDONG SI, QIANG LI, Brookhaven National Lab., CCNY/BNL TEAM — In recent years, the 2D-layered cobaltates have emerged as promising p-type thermoelectric materials due to their unique combinations of high thermo-coefficient and good metallic transport properties at ambient temperatures. These systems show high thermoelectric figure of merit and are ideal candidates as the materials of choice at elevated temperatures. We have carried out far-infrared magneto-spectroscopic studies of Ca$_3$Co$_2$O$_9$ thin films as a function of frequency, magnetic field and temperature with the emphasis on the coupling between the lattice, the charge and the spin degrees of freedom. The spectral response of this material is determined by the charge carriers and the polaronic field perpendicular or parallel to the CoO$_2$ layers. Below 20K, hysteresis occurs for perpendicular field but not for parallel field. This indicates that the negative magneto-resistance is due to reduced magnetic scattering when Co spins become aligned. Our results are consistent with co-existence of two types of carriers.

\textsuperscript{1}Supported by CUNY-RF-80209-11-13, DOE-AC02-98CH10886 and NSF-DMR-0451605.

3:18PM D28.00003 Direct measurement of charge transfer and spin state transitions in thermoelectric Ca$_3$Co$_2$O$_9$. GUANG YANG, University of Illinois at Chicago, QUENTIN RAMASSE, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, ROBERT KLINK, University of Illinois at Chicago — The misfit-layered thermoelectric material Ca$_3$Co$_2$O$_9$ has been the focus of many recent studies due to its high thermal power and good high temperature stability. In particular, it has been suggested that the presence of a mixed valence state in the strongly correlated CoO$_2$ layer is essential for the high p-type thermoelectric properties in Ca$_3$Co$_2$O$_9$. In this study, we combine aberration-corrected scanning transmission electron microscopy (STEM) with electron energy loss spectroscopy (EELS) to study the atomic and electronic structures of Ca$_3$Co$_2$O$_9$. We will show that the position of the O atomic columns in the CoO$_2$ layers are highly ordered and can therefore be directly imaged, while the CoO columns in the Ca$_2$Co$_2$O$_9$ rocksalt layer exhibit a strong modulation in the (010) direction. Further, we measure the local Co valence and find significant hole transfer from the rocksalt CoO to the strongly correlated CoO$_2$ layers. In addition, we will present the results of our in-situ heating experiments for power generation. The results of both substitutions will be discussed in light of recent first-principles electronic structure calculations. In the Sb-doped alloys, ZT was found to reach 0.5 at 1000 K and is projected to increase to 0.6 K at 1100 K, surpassing the industry standard for p-type materials as set by SiGe alloys.

3:30PM D28.00004 Thermoelectric properties of doubly doped Strontium Titanate thin films. JAYAKANTH RAVICHANDRAN, Applied Science and Technology Graduate Group, University of California, Berkeley, CA 94720, MATTHEW L. SCULLIN, Dept. of Materials Science and Engineering, University of California, Berkeley, CA 94720, SUBROTOM KUNERJEE, JOEL MOORE, Dept. of Physics, University of California, Berkeley, CA 94720, R. RAMESH, Dept. of Materials Science and Engineering, University of California, Berkeley, CA 94720, ARUN MAJUMDAR, Dept. of Mechanical Engineering, University of California, Berkeley, CA 94720 — Lanthanum doped Strontium Titanate (SrTiO$_3$) is amongst the most promising n-type thermoelectric materials for power generation. We report a double doping method for thin films of SrTiO$_3$, grown on (001) oriented LSAT substrates by Pulsed Laser Deposition (PLD), where doping of SrTiO$_3$ in the A-site by Lanthanum is accompanied by doping with oxygen vacancies. Based on careful transport measurements, we show that it is possible to obtain enhanced thermoelectric power factor in the limit of high effective mass and large carrier concentration in these thin films. The presence of oxygen vacancies also seems to decrease the thermal conductivity due to effective phonon scattering. The optimized doping concentration leads to a thermoelectric figure of merit, ZT > 0.2 at room temperature.

3:42PM D28.00005 Thermoelectric Properties and Band Structure Calculations of Novel Boron Network Compounds. TAKAO MORI, TOSHIYUKI NISHIMURA, National Institute for Materials Science (NIMS), YURI GRIN, Max Planck Institute for Chemical Physics of Solids, TOETSU SHISHIDO, KAZUO NAKAJIMA, Institute for Materials Research, Tohoku University — Boron is an interesting element, tending to form atomic networks such as 2D atomic nets and clusters, with some analogy to carbon systems which have been more extensively studied. Boron has less than an electron and thus is electron deficient when forming atomic networks, but this causes it to have a special affinity with the rare earth elements and as a result, many new compounds have recently been discovered \cite{1}. Their potential as viable thermoelectric materials is attracting interest since they have high thermoelectric materials and possess intrinsic low thermal conductivity, with some compounds exhibiting Seebeck coefficients in excess of 200 $\mu$V/K above 1000 K. The thermoelectric properties and band structure calculations of novel borides such as RB$_4$Si$_2$, RB$_7$CN, RB$_{22}$CoNi, RB$_{28}$Sc will be presented. Features in the band structure near the Fermi level indicate large doping effects in these compounds. Various doping experiments were carried out resulting in large increases to the figure of merit. [1] T. Mori, “Higher Borides,” in: Handbook on the Physics and Chemistry of Rare Earths, Vol. 38, (North-Holland, Amsterdam, 2008) p. 105-173.

3:54PM D28.00006 Electronic structure and high-temperature properties of doped Hf$_{0.5}$Zr$_{0.5}$CoSb phases. JACK SIMONSON, SLADE CULP, S. JOSEPH POON, University of Virginia, VIJAYABHARATHI PONNAMBAL, JUSTINE EDWARDS, TERRY TRITT, Clemson University — Half-Heusler alloys with compositions of the form Hf$_{0.5}$Zr$_{0.5}$CoSb were synthesized with Mn substituted to one or both of the Hf/Zr or Co sites or with the Sn site doped with Sn. The thermoelectric properties were evaluated from 300 K to 1000 K. The introduction of Mn was performed to investigate modifications to the band structure near the Fermi energy caused by transition metal substitution. Mn substitutions were discovered to increase the electrical resistivity dramatically while having no beneficial impact upon the thermopower. The Sb-doped alloys, on the other hand, exhibited lowered resistivity and thus increased efficiency of high temperature power generation. The results of both substitutions will be discussed in light of recent first-principles electronic structure calculations. In the Sb-doped alloys, ZT was found to reach 0.5 at 1000 K and is projected to increase to 0.6 K at 1100 K, surpassing the industry standard for p-type materials as set by SiGe alloys.

4:06PM D28.00007 Thermoelectric power generation in ternary skutterudites: a first-principles Wannier-functions\textsuperscript{1} study. DMITRI VOLJA, Massachusetts Institute of Technology, MARCO FORNARI, Central Michigan University, BORIS KOZINSKY, Bosch GmbH, NICOLA MARZARI, Massachusetts Institute of Technology — We study from first-principles ternary skutterudites derived from Co$_3$B$_8$, where the pnictogen is substituted with elements from the IVB and VIB groups. We focus on Co$_{2}$Ge$_{2}$As$_{2}$, Co$_{2}$Ge$_{2}$Te$_{2}$ and Co$_{3}$Sn$_{2}$Te$_{2}$, and compute the structure, electronic structure and vibrational properties from density-functional and density-functional perturbation theory. Since the direct evaluation of transport quantities in the relaxation-time approximation is computationally demanding, we use maximally-localized Wannier functions (MLWFs) for accurate integrations of operators across the Brillouin zone. This MLWFs basis leads to a very efficient and well-conditioned scheme to calculate the thermoelectric transport coefficients and to disentangle and identify the contribution of single bands. In addition, it provides a detailed, transferable picture of bonding in these complex materials.

4:18PM D28.00008 Thermoelectric Properties in Nanostructured p-type Skutterudites. XIAO YAN, Boston College, QING HAO, Massachusetts Institute of Technology, JIAN YANG, HUI WANG, YUCHENG LAN, DEZHI WANG, Boston College, GANG CHEN, Massachusetts Institute of Technology, ZHIFENG REN, Boston College, BOSTON COLLEGE COLLABORATION, MASSACHUSETTS INSTITUTE OF TECHNOLOGY COLLABORATION — Skutterudites are good examples of phonon glass electron crystal (PGEC), which is proposed to be one of the most desirable materials to maximize the thermoelectric figure of merit. The skutterudite structure has two voids in each unit cell that are large enough to accommodate a variety of atoms, such as La, Ce, Nd, Sm, Yb, etc. These atomic void-fillers rattle about in their oversized cages, thereby drastically reducing thermal conductivity and maximizing ZT. Our work on p-type skutterudites is based on compounds of a general formula FeRh$_{3}$Co$_{5}$Sb$_{2}$, which stands for a void filler. Besides the influence of rattling of the void fillers, thermal conductivity can be further depressed by the increased phonon scattering at the increased grain boundaries due to nano size grains.
4:30PM D28.00009 Calculation of electric field gradients and site preference in Ba-Al-Ge clathrates, SERGIO RODRIGUEZ, WEIPING GOU, JOSEPH ROSS, Texas A&M University — Sn, Ge or Si can form cage-like clathrate structures, many of which exhibit enhanced thermoelectric performance. To understand Al substitutional occupation in $\text{Ba_xGa_{16-x}Si_xGe_{30-x}}$ Clathrates we performed NMR lineshape simulations for $3 \leq x \leq 24$, and $0 \leq y \leq 3$, where $\square$ represents a vacancy. The electric field gradient (EFG) was calculated for Al sites assuming an ordered structure. To obtain the EFG we used ab initio methods in the Generalized Gradient Approximation as implemented by the WIEN2k code with structural relaxation. Results where used to simulate NMR lineshapes numerically. These were compared to our previously reported NMR lineshapes. For fully occupied $\text{Ba_xGa_{16-x}Al_y}$ we compare different site occupations, obtaining good agreement and thus information about Al site preferences. For reduced-Al samples, WDS measurements indicate the presence of spontaneous vacancies. In the case of the Zintl phase $\text{Ba_xGa_{16-x}Al_{y+x}}$, we found that Al sites adjacent to the vacancy exhibit a large EFG, while those with the vacancy further away have smaller EFG's. Assuming a larger Knight shift for sites next to vacancies, we obtain good agreement with NMR experimental results for reduced-Al $\text{Ba_xGa_{16-x}Al_{y+z}}$. We infer that Al prefers locations close to vacancies rather than random occupation. Supported by Robert A. Welch Foundation (Grant A-1526).

4:42PM D28.00010 The effects on the electronic properties of the clathrates $\text{A_xGa_{16}Si_xGe_{30-x}}$ ($A=\text{Ba, Sr}$), EMMANUEL NENGHABI, CHARLES MYLES, Texas Tech University — We have studied the structural and electronic properties of the Ba and Sr guest-containing type-I semiconductor clathrates $\text{Ba_xGa_{16}Si_xGe_{30-x}}$ and $\text{Sr_xGa_{16}Si_xGe_{30-x}}$ for Si compositions $x = 0, 5$ and $15$. Our calculations are based on the general gradient approximation (GGA). Starting with stable structures of the Ge-based type I clathrate semiconductors $\text{Ba_xGa_{16}Ge_{30-x}}$ and $\text{Sr_xGa_{16}Ge_{30-x}}$ containing no Ga-Ga bonds, we have constructed unit cells of $\text{Ba_xGa_{16}Si_xGe_{30-x}}$ and $\text{Sr_xGa_{16}Si_xGe_{30-x}}$ by replacing appropriate number of the framework Ga atoms with Si. For the values of $x$ that we have considered, we find that the fundamental band gap of $\text{Ba_xGa_{16}Si_xGe_{30-x}}$ increases with increasing $x$ but that the band gap of $\text{Sr_xGa_{16}Si_xGe_{30-x}}$ increases with increasing $x$. We also find that several electronic states near the top of the valence band and near the bottom of the conduction band in both materials are modified by the Si p states. The trends in the structural and electronic properties of Si are varied and discussed, and our results are compared to experiment where possible.

5:06PM D28.00012 Large Thermolectric power factor in CrN, CAMILO QUINTELA, Applied Physics Department, University of Santiago de Compostela, 15782-Santiago de Compostela, Spain, FRANCISCO RIVADULLA, Physical Chemistry Department, University of Santiago de Compostela, 15782-Santiago de Compostela, Spain, JOSE RIVAS, Applied Physics Department, University of Santiago de Compostela, 15782-Santiago de Compostela, Spain. — We report the electrical resistivity and thermoelectric power of stoichiometric and hole-doped chromium nitride (CrN). The results indicate a considerably large power factor, of the order of 1(microW/cmK2) at 400 K, increasing with temperature. Hall effect measurements were used to elucidate the mechanism of electronic transport in this system, in order to optimize its properties. The easy of grow in the form of nanoparticles and thin films, along with a good thermal stability up to 700 K, could make this material interesting for applications at moderate temperatures.

Monday, March 16, 2009 2:30PM - 5:30PM Session D29 Fed: Focus Session: The Physics and Astronomy New Faculty Workshops I

2:30PM D29.00001 A Dozen Years and a Thousand Participants: The Workshops for Preparing New Faculty in Physics and Astronomy¹, KENNETH KRANE, Department of Physics, Oregon State University, Corvallis OR 97331 — Beginning in 1996, an annual workshop for newly hired faculty in physics and astronomy has been held under the organizational leadership of AAPT, APS, and AAS. To date more than 1000 faculty have participated in this workshop, representing approximately 25% of the new hires at all U. S. institutions that award a baccalaureate in physics or astronomy, from 4-year colleges through research universities. The original motivation for the workshops was to improve physics teaching by introducing new faculty to instructional strategies and innovations that had been shown to be effective in a variety of contexts. The need for such a program was suggested in part by the belief that a national mentoring workshop could effectively address a commonality of physics and astronomy teaching challenges that transcended institutional characters and types, and also in part by the reaction to a significant decrease in the number of baccalaureate physics degrees awarded in the U. S. in the 1990s, which many believed was due to ineffective and uninspiring teaching at the undergraduate level and especially in introductory courses. Based on surveys of the participants (and their department chairs), we have found that a large fraction of the participants have become adopters of innovative teaching techniques and that they rate the workshops as the most significant cause of the improvements in their teaching. This talk will summarize the development of the workshop program since its inception, the measures of its success in improving teaching, and the plans for its future.

¹Supported in part by NSF DUE grants 9554738 and 0121384.

3:06PM D29.00002 Teaching New Dogs New Tricks: The Next Generation of Physics Faculty, GERALD FELDMAN, George Washington University — I was privileged to attend the first New Faculty Workshop (NFW) in 1996, and that was the spark that kindled my keen interest in teaching methodology, learning assessment, and Physics Education Research (PER). Following Eric Mazur’s introduction to Peer Instruction, I became a strong advocate of ConcepTests in class, implemented an electronic student response system before they were widely in vogue, and emphasized conceptual understanding on the same footing as numerical computations. This led to a research project on the efficacy of in-class ConcepTests, and further, to the linking of conceptual and numerical aspects in a “thinking skills” curriculum for introductory physics at George Washington University (Gwu). After “dabbling” in PER for some years, several of us at GWU now have a credible research program and our first Ph.D. student in PER. The methods espoused by PER have extended to other members of the Physics Department, and even beyond, to other science departments on campus. Following this trend, we have most recently (Spring 2008) implemented a SCALEUP collaborative classroom modeled after the work of Bob Beichner at NC State. Overall, the teaching climate in the GWU Physics Department has changed considerably over the past decade, and it is clear that these changes ultimately trace their origins back to the impact of the NFW on the faculty members who have attended over the years.

3:18PM D29.00003 Effects of the New Faculty Workshop at WFU, FREDDIE SALSIBURY, Wake Forest University — Two members of the Wake Forest University Physics department have attended the Physics and Astronomy New Faculty Workshop and have implemented many of the lessons learned in their classes and in the department. In particular, the impacts on teaching introductory and upper-level physics, and developing a biophysics track will be discussed.
3:30PM D29.00004 Twenty semesters later: how NFW helped us to multiply majors. A. ALAN MIDDLETON, Syracuse University — In the Fall of 1997, I missed my daughter’s first Halloween to attend the NFW. Though that was disappointing, I was pleasantly surprised to learn that there were a number of people who thought about teaching and had very constructive ideas to share. I immediately applied what I had learned in the large lecture class that I taught for a few years, with success for my students and my career. I then spent 7.5 years as the Director of Undergraduate Studies: the contacts and insights provided by the NFW and subsequent occasional attendance at AAPT meetings were most helpful in improving our program (the number of graduating majors increased from about 3 to over 15 per year), along with the help of a few dedicated faculty at Syracuse. The specific pedagogical viewpoints and tools introduced at the NFW were helpful in my teaching and administrative work, but the most useful part of the experience was the license granted to seek improvements in both teaching and the undergraduate program and provide contact with others who took such issues seriously.

3:42PM D29.00005 The Best of Both Worlds, ELIZABETH H. SIMMONS, Michigan State University — Thanks to the New Faculty Workshop, I now have dual identities: as a professor in a research-focused university physics department and as Dean of a teaching-focused undergraduate residential science college within that university (Lyman Briggs College). I’ll talk first about how the NFW changed my perspective on education and outreach — and how that affected the climate in the department I was in at the time. Next, I’ll comment on how this shift of perspective eventually led to new professional opportunities, including my current dual position. The lessons from the NFW have contributed directly to my acquiring the skills required of a leader in an interdisciplinary college that encourages its faculty both to be active disciplinary researchers and to take a scholarly approach to teaching. Finally, I’ll mention how being part of the college’s community of teacher-scholars has helped my teaching to continue evolving in directions compatible with the aims of the New Faculty Workshop.

3:54PM D29.00006 ReDUCE: Rethinking Directions in Undergraduate Curriculum Experiences, CARLOS WEXLER, DEBORAH HANUSCIN, MATTHEW MOWER, HASKELL TAUB, University of Missouri — There is a major emphasis in higher education on rethinking undergraduate science instruction, particularly in introductory courses. In Fall/2007 a collaborative team at the University of Missouri formed and was given a “green light” to start an overhaul of the curriculum and instruction of (algebra-based) Physics I and the associated laboratory/recitation, a course taken by > 500 students/yr. Earlier, we had identified problems with the current status of the course: the number of topics “crammed into the syllabus,” disconnection of laboratories to each other, and lack of conceptual coherence between laboratory, recitations and lectures. In Spring/2008, the group was awarded an interdepartmental grant from the College of Education to begin work on realigning the lecture, lab, and recitation components of the course around a coherent curriculum that builds towards “big ideas” in the discipline (a “narrow but deep” approach). In Fall/2008 we implemented the first pilot test by combining exploratory labs, “take-home-mini-labs,” and the use of Tutorials (in one section of the lab of this course, ca. 20 students). In this talk I will discuss early results and conclusions of this experiment, the next steps in the academic transformation, funding issues, and hurdles faced towards implementation on larger scale.

4:06PM D29.00007 JiTT and Peer Instruction in the General Physics Sequence at Dominican College: A One-Year Retrospective, KATHLEEN HINGE, Dominican College — Energized by the New Faculty Workshop of November, 2007, the author returned to Dominican College of Blauvelt with dreams of colossal gains on Force Concept Inventory (FCI) scores. Replicating the reported successes at Harvard and the US Air Force Academy would be difficult at Dominican: More than one-third of Dominican’s physics students are minority, and an even greater portion of students come from secondary education without the ability to synthetically apply concepts. Undeterred, the author was committed to overthrowing the General Physics sequence around NFW tenets. Beginning in January, 2008, material presentation went from traditional lecture format to a combination of Just in Time Teaching (JiTT) and Peer Instruction. This paper presents a one-year retrospective on this process, with emphasis on lessons learned, the impact on student learning and satisfaction, and next steps. Student response to the change has been uniformly enthusiastic. The actual FCI gain achieved in this first year was G=0.31, a modest advance over the 0.25 reported for traditionally taught courses. Spurred by this early success, implementation of JiTT has spread to courses in Biology and Mathematics.

4:18PM D29.00008 A Tale of Two Curricula: The performance of two thousand students in introductory electromagnetism, MICHAEL SCHATZ, MATTHEW KOHLMYER, MARCOS CABALLERO, School of Physics, Georgia Institute of Technology, RUTH CHABAY, BRUCE SHERWOOD, Department of Physics, North Carolina State University, RICHARD CATRAMBONE, MARCUS MARR, School of Psychology, Georgia Institute of Technology, MARK HAUGEN, Department of Physics, Purdue University, LIN DING, Department of Physics, The Ohio State University — Student performance in introductory calculus-based electromagnetism (E&M) courses at four large research universities was measured using the Brief Electricity and Magnetism Assessment (BEMA). Two different curricula were used at these universities: a traditional E&M curriculum and the Matter & Interactions (M&I) curriculum. At each university, post-instruction BEMA test averages were significantly higher for the M&I curriculum than for the traditional curriculum. The differences in post-test averages cannot be explained by differences in variables such as pre-instruction BEMA scores, grade point average, or SAT scores.

4:47PM D29.00009 Improving clicker questions for enhanced learning in the interactive physics classroom, ERTAN SALIK, Cal Poly Pomona — Classroom response systems, or clickers, have become widely used in physics classes in the last decade. Physics education research has demonstrated clearly that it is not the clicker as an electronic tool, but the interactive learning that occurs through clickers is what improves student learning. For clickers to work as expected, however, many subtle details need to be addressed. An instructor can start using many questions developed for the purpose of peer instruction. For a particular student population, and for a particular learning environment and constraints of the educational institution, questions used and the instructor’s teaching style may need to be altered over time. We will present a systematic way of improving clicker questions and one’s own teaching style utilizing data collected during clicker sessions. In addition, by adding a small writing component to some clicker questions, one can simply peek into student reasoning in order to determine preconceptions and misconceptions. Such direct knowledge of student reasoning in one’s own class may be very revealing, and help improve learning ultimately.

1Supported by NSF DUE.

3:30PM D29.00009 Improving clicker questions for enhanced learning in the interactive physics classroom, ERTAN SALIK, Cal Poly Pomona — Classroom response systems, or clickers, have become widely used in physics classes in the last decade. Physics education research has demonstrated clearly that it is not the clicker as an electronic tool, but the interactive learning that occurs through clickers is what improves student learning. For clickers to work as expected, however, many subtle details need to be addressed. An instructor can start using many questions developed for the purpose of peer instruction. For a particular student population, and for a particular learning environment and constraints of the educational institution, questions used and the instructor’s teaching style may need to be altered over time. We will present a systematic way of improving clicker questions and one’s own teaching style utilizing data collected during clicker sessions. In addition, by adding a small writing component to some clicker questions, one can simply peek into student reasoning in order to determine preconceptions and misconceptions. Such direct knowledge of student reasoning in one’s own class may be very revealing, and help improve learning ultimately.

1Cal Poly Pomona Faculty Center for Professional Development
4:42PM D29.00010 Propagations of the AAPT New Faculty Workshop: A case study of the infusion of student-centered technological and pedagogical innovations in the introductory physics program at West Point, BRYNDOL SONES, US Military Academy — Since 2002, the Department of Physics at West Point has been the fortunate recipient of yearly attendance at the AAPT New Faculty Workshop. This sustained involvement has contributed directly to enhancements in our two-semester introductory physics program. Two aspects of West Point’s environment make our involvement with the workshop especially fruitful: our diverse students and our frequent faculty turn-over. We teach to over 1100 students with majors across the entire spectrum. The majority of our faculty is an active duty Army officer here for just three years. At West Point, we rely on the workshop as a wellspring for faculty development, technological innovation, and pedagogical refinement. In the past few years, we have incorporated aspects of peer instruction, activity-based learning, and tutorials for student discovery. On the technological side, we now have TabletPCs for faculty, rf response cards (TurningPoint), high speed video analysis (LoggerPro) projects, and video tutoring capabilities (Camtashia). Student achievement is measured through our traditional course evaluation tools as well as nationally recognized standardize tests. Results will be discussed in the presentation.

4:54PM D29.00011 Instilling best educational practices into future physics professionals and faculty, PHILIP G. COLLINS, Department of Physics and Astronomy, Univ. of California Irvine, Irvine CA 92697-4576 — A primary aim of the New Faculty Workshop (NFW) has been to communicate best educational practices in faculty beginning their teaching careers. However, further amplification of NFW goals is achieved by providing similar content and training to Ph.D. candidates working as Teaching Assistants (TAs). NFW experience led to the successful creation at UCI of a relatively extensive, 30-hour training course now required of every graduate student in the Dept. of Physics and Astronomy. Half of the training occurs before the first week of classes, and focuses on peer instruction, active learning, and results from Physics Education Research. This orientation segues into peer evaluation as first-time TAs and soon-to-be TAs practice teaching styles for each other and evaluate videos of each other teaching their actual courses. This course directly trains 25-30 graduate students each year, indirectly affecting dozens of discussion sections and the experience of nearly 2000 students per quarter.

5:06PM D29.00012 Applying New Faculty Workshop Lessons to Intermediate-Level Physics Courses, MELISSA EBLEN-ZAYAS, Carleton College — Although much innovative work on physics teaching techniques and curriculum has been carried out at the level introductory physics resources, there has been less focus on the intermediate-level physics courses. Since my participation in the new faculty workshop, I have been particularly interested in finding ways to implement peer instruction and other active learning strategies in sophomore and junior level physics classes. Many curricular resources are available for introductory physics, but finding appropriate materials for courses beyond the introductory level is more challenging. I will discuss the use of comPADRE resources as well efforts to develop original activities to promote active learning and conceptual understanding, and I will highlight the successes and challenges of integrating these types of activities in intermediate-level physics courses.

5:18PM D29.00013 From Syllabus To Diagnostic Exam: Learnings from the New Faculty Workshop Applied into the Intro Physics Classroom, MICHAEL TANOFF, Kalamazoo College — Kalamazoo College offers a “one-size-fits-all” concept-based introductory physics sequence. The widely varying demographic composition of the class — including majors in biology, chemistry, pre-med, physics, and math, along with occasional humanities majors — adds obvious challenges to the successful learning experience. As such, educational techniques that apply across the demographic are required. Several ideas presented at the Fall 2005 New Faculty Workshop apply to the needs of this broad range of students at Kalamazoo College, including an “organic” course syllabus that has been allowed to grow to whatever extent necessary to address student concerns and misunderstandings about course expectations, policies, and guidelines, and to provide advice on recurring themes; peer instruction for maximizing classroom value; and hiring teaching assistants with first hand experience in the course and the labs. Details on implementing these techniques, including developing a syllabus with unusual section headings such as “Attendance and Homework Dramas” and “Introductory Physics Survival Requirements,” will be presented. Success of the techniques, as evidenced by performance on diagnostic exams, class attendance, and comments from course evaluations, will be discussed.

Monday, March 16, 2009 2:30PM - 5:30PM —
Session D30 DMP GMAG: Focus Session: Cobaltite and Manganite films 334

2:30PM D30.00001 Emergent Phenomena in Spatially Confined Manganites, THOMAS WARD, University of Tennessee & Oak Ridge National Laboratory — There is evidence that chemically disordered single crystal manganites exhibit electronic inhomogeneity in which areas with vastly different electronic and magnetic properties form and coexist in phase separated domains ranging in size from a few nanometers to micrometers. This phase separation is of particular interest, as it has been suggested that it is the central feature that leads to colossal magnetoresistance in manganites, the Mott transition in VO2 and may play a part in high-TC superconductivity in cuprates. We will discuss our ongoing efforts to answer fundamental questions about the specific role of PS in complex oxides using a novel spatial confinement technique. Unlike transport measurements on bulk or thin films where the electrons follow only the metallic path of least resistance, spatially confining a phase separated material to the scale of its inherent domains forces electrons to travel through both the metallic and insulating regions that lie along the conduction path. This has led to observations of several new phenomena such as a reemergent metal-insulator transition, ultra-sharp jumps in resistivity at the metal-insulator transition, and the first high resolution observation of stable single domain electronic phase transitions in time. La(5/8-x)Pr(x)Ca(3/8)MnO(3) (LPCMO) is used as a model system due to its large scale electronic phase separation into ferromagnetic metal (FM) and charge ordered insulator (COI) electronic phase domains and well documented spin-charge-lattice interactions. These properties allow us to isolate domains through conventional wet etch techniques and offer a wide range of tunability through doping and substrate strain. This ability to control key elements of the underlying complexity and observe the resulting changes in the emergent behavior help answer questions about the fundamental physics that rule complex materials.

3:06PM D30.00002 Electric field induced anisotropic transport properties of phase separated (La(1-x)Pr(x))0.67Ca0.33MnO3 thin films1, HYOUNG JEEN JEEN, ALESSANDRA GALLASTEGUI, AMLAN BISWAS, Department of Physics, University of Florida, Gainesville, Florida 32611 — The perovskite manganese oxide (La1−xPrx)0.67Ca0.33MnO3 thin films exhibit electronic phase separation i.e., a ferromagnetic metallic phase and a charge ordered insulated phase coexist in a certain temperature range. It was shown that in such a phase separated state thin films of manganites show a colossal magnetoresistance (CER) although the mechanism driving this phenomenon is still unknown. We present transport measurements which show that the CER is due to an electric field driven anisotropy in phase separated manganites. LPCMO thin films were grown on NdGaO3 (110) substrates using Pulsed Laser Deposition. A cross shaped micro-structure, with 60 by 10 µm legs, was fabricated using UV photolithography and chemical etching. We observe CER close to the insulator to metal transition temperature (Tc) in the longitudinal direction i.e. parallel to the applied electric field. We simultaneously measure the transverse resistance in the other (orthogonal) leg of the microstructure. We observe a clear anisotropy in the conduction of the cross shaped microstructure which could be the origin of CER in manganites.

1Supported by NSF DMR-0804452
3:18PM D30.00003 Colossal electroresistance in phase separated manganite nanobridges1, G. SINGH-BHALLA, A. BISWAS, A. F. HEBARD — We have examined the electric field effect on the nanometer scale in the manganite (La$_{1-y_3}$/Pr$_y$)MnO$_3$ thin films. The interfacial strain between the ferromagnetic (FM) and antiferromagnetic (AFM) phase is obtained by first principles and consistent with each fully-optimized atomic structure at different pressures. With structurally invariant dielectric response, we show that atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy in combination with ab-initio first-principles DFT calculations can be utilized to measure the spin-state transition in the current-voltage characteristics implying either a change in resistance arising from spin canting or a change in the ferromagnetic phase fraction. Next, within the micrometer scale PS temperature regime, current-voltage measurements reveal colossal, step-like drops in resistance with increasing current. We will discuss our results both in the context of previously considered models for manganite electroresistance and new interpretations with a focus on the microscopic details of the metallic and insulating regions.

1Work supported by NSF grant DMR-0704240 and DMR-0804452

3:30PM D30.00004 Phase modification of La$_{1/4}$Pr$_{3/4}$Ca$_3$MnO$_3$ thin films by light, magnetic field and applied stress1, JUSTIN OLAMIT, MIKHAIL ZHERNENKOV, MIKE FITZSIMMONS, Los Alamos National Laboratory, HAILE AMBAYE, VALERIA LAUTER, Oak Ridge National Laboratory, HYOUNG JEEN JEEN, AMLAN BISWAS, University of Florida — Complex oxide materials exhibit a wide variety of fascinating electromagnetic properties related to the coexistence of multiple electric and magnetic phases. The temperature-magnetic field phase diagram of La$_{27}$Pr$_{40}$Ca$_{33}$MnO$_3$ (LPCMO) is intriguing; a ferromagnetic metallic (FM) phase, charge ordered insulating (COI) phase, and conditions where both phases coexist are accessible with changes in temperature and magnetic field. We have performed neutron reflectometry to understand the emergence of the FMF phase in a COI matrix of a LPCMO thin film as functions of temperature, irradiation with light, magnetic field and stress. Specular reflectivity reveals the emergence of ferromagnetism below the phase transition temperature. Diffuse scattering shows that the length scale of FM domains is 1-2 microns. [1] Ch. Renner et al., Nature 416, 518 (2002). [2] L. Zhang et al., Science 298, 805 (2002). [3] T. Dhakal et al., Phys. Rev. B 75, 092404 (2007).

Work supported by DOE Contract DE-AC52-10NA27396.

3:42PM D30.00005 Real-Space Imaging of Electronic Phase Separation in a Mn-Doped Bilayered Ruthenate1, TAE-HWAN KIM, M. ANGST, R. JIN, X.G. ZHANG, J.F. WENDELKEN, A.P. LI, Oak Ridge National Laboratory, B. HU, E.W. PLUMMER, The University of Tennessee — Transition-metal oxides with multiple nearly degenerate states show very complicated phase diagrams. Small perturbations can often dramatically change their functionalities. It is believed that electronic phase separations (PS) play an important role in the exotic functionality. Direct experimental observation of PS has thus become crucial to understanding underlying mechanisms of the striking functionalities. We have studied the PS and the evolutions of phase domains with temperature near the Mott transition in a Mn-doped bilayered ruthenate Sr$_5$(Ru$_{1−x}$Mn$_x$)$_2$O$_7$. Our experimental approach combines electron microscopy, scanning tunneling microscopy, and electron transport spectroscopy, which provide unprecedented capabilities of imaging PS and interrogating individual microscopic domains in situ. A quantitative correlation has been determined between the macroscopic metal-insulator transition and the microscopic phase domain percolation in Sr$_5$(Ru$_{1−x}$Mn$_x$)$_2$O$_7$.

1The research at Oak Ridge National Laboratory was sponsored by the Scientific User Facilities Division and the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. DOE.

3:54PM D30.00006 Mapping the phase boundaries in thin-film manganites using scale-invariant dielectric response1, P. MICKEL, G. SINGH-BHALLA, S. TONGAY, A. BISWAS, A. F. HEBARD, University of Florida — Magneto-capacitance techniques have been used in a study of (La$_{1−x}$Pr$_x$)$_3$Ca$_3$MnO$_3$ (LPCMO) thin films to determine the range of phase space, described by frequency ($\omega$), temperature (T) and field (H), over which a dielectric response of the form, C($\omega$,T,H) = [C($\omega$,T,H) - C$_0$]$^{1/\gamma}$, is found to hold. This power-law scaling collapse (PLSC) of the complex capacitance (C), expressed in a Cole-Cole formulation, differs from the well-known "universal" dielectric response (UDR), where the exponent $\gamma = 1$. The influence of film thickness and stoichiometry on the extent of the PLSC region is investigated with the implementation of a new phase-space mapping technique. The mappings clearly illustrate the onset of phase competition in LPCMO, delineating boundaries which correspond to capacitive minima at low temperatures, where the first-order insulator-metal transition occurs, and to the second-order paramagnetic-insulator/charge-ordered-insulator transition at higher temperatures, where a resistive transition signature exists in bulk but not in thin films. Modeling with distributions of UDR elements corresponding to the different manganese phases gives a good qualitative account of the observed behavior, and can lead to the determination of individual phase fractions.

4:06PM D30.00007 Direct measurement of the low-temperature spin-state transition in epitaxially strained LaCoO$_3$ thin films, ROBERT KLIE, GUANG YANG, YUAN ZHAO, Department of Physics, University of Illinois at Chicago — The perovskite oxide LaCoO$_3$ exhibits an anomaly in its magnetic susceptibility at 80 K associated with a thermally excited transition of the Co$^{3+}$-ion spin. We will show that atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy in combination with ab-initio first-principles DFT calculations can be utilized to measure the spin-state transition in LaCoO$_3$. In particular, we utilize in-situ cooling experiments in a transmission electron microscope to demonstrate that the O K edge pre-peak is sensitive to the Co$^{3+}$-ion spin-state. Our experimental results will be compared to first-principles calculations, and we will conclude that the thermally excited spin-state transition occurs from a low to an intermediate spin state, which can be distinguished from the high-spin state. Next, we will examine the effects of biaxial strain and point defects in LaCoO$_3$ thin-films on the Co$^{3+}$-ion spin-state. We will show that a single-crystal pseudo-cubic LaCoO$_3$ (001) film can be successfully grown on LaAlO$_3$ (001). Moreover, we will show that the epitaxially strained LaCoO$_3$ film exhibits a ferro-magnetic transition at the current level that was not observed in bulk LaCoO$_3$. We will discuss the origin of this transition and the possibility of stabilizing different Co$^{3+}$-ion spin-states in LaCoO$_3$ using interfacial strain.

4:18PM D30.00008 First-principles study for low-spin LaCoO$_3$ with structurally consistent Hubbard $U$, HAN HSU, KOICHIRO UMEMOTO, MATTEO COCOCCIONI, RENATA WENTZCOVITCH, Chemical Engineering and Materials Science, University of Minnesota — We use the local density approximation + Hubbard $U$ (LDA+U) method to calculate the structural and electronic properties of low-spin LaCoO$_3$. The Hubbard $U$ is obtained by first principles and consistent with each fully-optimized atomic structure at different pressures. With structurally consistent $U$, the fully-optimized atomic structure agrees with experimental data better than the calculations with fixed or vanishing $U$. A discussion on how the Hubbard $U$ affects the electronic and atomic structure of LaCoO$_3$ is also given.

1This work was supported primarily by the MRSEC Program of the National Science Foundation under Award Number DMR-0212302 and DMR-0819885, and supported partially by the NSF/ITR program through the University of Texas (ITAMIT).
4:30PM D30.00009 Direct observation of local magnetic properties in strain engineered lanthanum cobaltate thin films. S. PARK, WEIDA WU, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA; J. W. FREELAND, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA; J. X. MA, J. SHI, Department of Physics, University of California, Riverside, California 92521, USA — Strain engineered thin film devices with emergent properties have significant impacts on both technical application and material science. We studied strain-induced modification of magnetic properties (Co spin state) in epitaxially grown lanthanum cobaltate (LaCoO$_3$) thin films with a variable temperature magnetic force microscopy (VT-MFM). The real space observation confirms long range magnetic ordering on a tensile-strained film and non-magnetic low-spin configuration on a low-strained film at low temperature. Detailed study of local magnetic properties of these films under various external magnetic fields will be discussed. Our results also demonstrate that VT-MFM is a very sensitive tool to detect the nanoscale strain induced magnetic defects.

4:42PM D30.00010 Understanding the Origin of Ferromagnetism in Strained LaCoO$_3$ Thin Films. J.X. MA, J. SHI, Department of Physics, University of California at Riverside, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory — Using strain to control the behavior of strongly correlated materials offers new opportunities to control fundamental properties. For the case of magnetism, LaCoO$_3$ offers the ability to use strain through thin film growth to manipulate directly the spin-state of Co in this system. Here we present the results of a detailed polarized x-ray spectroscopy study of LaCoO$_3$ thin films grown on SrTiO$_3$(001) and LaAlO$_3$(001) substrates. X-ray diffraction from 25 nm thin films confirms the films are fully strained in both cases and, for films under tensile strain, total moment magnetometry shows a clear transition to ferromagnetic state at ≈0.6 Tesla. X-ray absorption shows that the films grown from a LaCoO$_3$ target are slightly hole doped due to non-stoichiometry generated during growth (effective doping ≈0.1 holes per unit cell), which in the bulk is sufficient to destroy the low-spin state. However, even though the films are slightly hole doped, the films under tensile strain show long range ferromagnetic order unlike the bulk system. Since the films are insulating, these results are consistent with a ferromagnetic insulating state arising due to superexchange. Work at UCR is supported by ONR/DMEA under award H94003-08-2-0803.

4:54PM D30.00011 Structure, Magnetism, and Transport in SrTiO$_3$(001) / La$_{1-x}$Sr$_x$CoO$_3$: Evidence for Interfacial Magnetic Phase Separation. M.A. TORJIA, M. SHARMA, C. HE, Univ. of Minnesota, J. GAZQUEZ, M. VARELA, ORNL, M. LAVER, B.B. MARANVILLE, J.A. BORCHERS, NIST, C. LEIGHTON, Univ. of Minnesota — Doped cobaltites have proven to be excellent choices for the study of the magneto-electronic phase separation phenomenon. Strong motivation exists for the study of these materials in films and heterostructures, the effect of dimensional confinement on this phase separation being a prime example. We investigated the structure, magnetism, and magnetotransport, in epitaxial La$_{1-x}$Sr$_x$CoO$_3$ on SrTiO$_3$(001). We have observed deterioration in ferromagnetism and conductivity in the thin film limit (e.g. < 8 nm at x = 0.5). We demonstrate that this can be definitively ascribed to interfacial magnetoelectronic phase separation. Key observations are the existence of an intercluster "GMR", anomalous multiterminal transport, strongly non-gaussian resistance fluctuations, and direct measurement of short-range ferromagnetic order by SANS. The thickness of the phase-separated region diverges as the doping is reduced from x = 0.50 to x = 0.18, and it can also be induced by deposition of SrTiO$_3$ overlayers. STEM/EELS data rule out the possibility of chemical phase separation proving that the deterioration in magnetic and electronic properties near the interface with SrTiO$_3$ is due to an intrinsic magnetic phase separation effect. [Supported by NSF and DOE].

5:06PM D30.00012 Electronic structure of La$_{1-x}$Sr$_x$CoO$_{3-\delta}$ in the presence of ordered oxygen vacancies$^1$. JAUME GAZQUEZ, M. VARELA, Oak Ridge National Laboratory, M.P. OXLEY, W. LUO, S.T. PANTLEIDES, Vanderbilt Univ., M.A. TORJIA, M. SHARMA, C. LEIGHTON, Univ. of Minnesota, S.J. PENNYCOOK, Oak Ridge National Laboratory — Here we present a study of oxygen vacancy ordering in La$_{1-x}$Sr$_x$CoO$_{3-\delta}$ (LSCO) thin films using a combination of atomic resolution Z-contrast imaging and electron energy-loss spectroscopy (EELS). Substituting Sr for La in LSCO results in either the formation of oxygen vacancies or an increase in the mean cobalt valence in order to preserve charge neutrality. At large concentrations, oxygen vacancies in LSCO form ordered structures with orientations determined by epitaxial strain. This talk will show how different O K-edge fine structures can be observed in EEL spectra obtained from different sites of the superstructure, while the Co L-edges are unchanged. These results, together with density functional theory and dynamical scattering calculations, suggest that there is no charge ordering but a modulation of the effective density of states in these systems.

5:18PM D30.00013 Magnetic phase separation-induced coercivity enhancement in epitaxial Nd$_{0.5}$Sr$_{0.5}$CoO$_3$ films$^1$. M. SHARMA, M. VARELA, ORNL, J. GAZQUEZ, M. VARELA, ORNL, C. LEIGHTON, ORNL — Interfacial magneto-electronic phase separation has recently been observed in epitaxial thin films of the doped perovskite cobaltite La$_{1-x}$Sr$_x$CoO$_3$ at doping values where no such phase separation exists in bulk. Such systems also display anomalously large coercivity, which is not understood. To achieve a better understanding of this phenomenon we have extended this study to Nd$_{0.5}$Sr$_{0.5}$CoO$_3$ (x = 0.5), the perovskite cobaltite with the largest coercivity in bulk. Thin films of Nd$_{0.5}$Sr$_{0.5}$CoO$_3$ are grown via high pressure reactive sputtering on SrTiO$_3$(001) substrates. We have observed a rapid deterioration in magnetization and onset of large intercluster-type magnetoresistance below a critical thickness of 80 Å. Signatures of interfacial magneto-electronic phase separation also seen in our earlier work on La$_{1-x}$Sr$_x$CoO$_3$. The temperature, angular, and thickness dependence of the coercivity ($H_c$) was studied using magnetoresistance. Low temperature $H_c$ values become very large (up to 3.6 Tesla) at low thickness, and a strong, superlinear $T$ dependence emerges. We propose that the coercivity enhancement arises due to efficient domain wall pinning by the inhomogeneously magnetically phase separated region near the SrTiO$_3$ substrate.

$^1$Work supported by NSF and DoE.

Monday, March 16, 2009 2:30PM - 5:30PM
Session D31 GMAG: Focus Session: Quantum Magnets 335

2:30PM D31.00001 Spin Relaxation in Pure and Doped GGG. MICHAEL SCHMIDT, THOMAS ROSENBAUM, DANIEL SILEVITCH, University of Chicago, GABRIEL AEPPLI, University College London, SAYANTANI GHOSH, Y.K. VERMA, University of California, Merced — Geometric frustration in Gadolinium Gallium Garnet (GGG) leads to local regions of correlated spins that can be manipulated without affecting the background spin susceptibility. These “quantum protectorates” can be accessed via the non-linear response at milliKelvin temperatures using a hole burning technique. We study the effect of impurities on both the structure of the spin clusters and the dissipation spectrum in Neodymium-doped GGG crystals via pump-probe ac magnetic susceptibility and direct optical measurements.
2:42PM D31.00002 Bose-Einstein Condensation of Triplons in Ba$_3$Cr$_2$O$_6$\textsuperscript{1}, A.A. ACZEL, McMaster University, Y. KOHAMA, M. JAIME, Los Alamos National Laboratory, L. BALICAS, National High Magnetic Field Laboratory, K. NINIOS, H.B. CHAN, University of Florida, H.A. DABKOWSKA, G.M. LUKE, McMaster University — By performing heat capacity, magnetocaloric effect, torque magnetometry and force magnetometry measurements up to 33 T, we have mapped out the T-H phase diagram of the S = 1/2 spin dimer compound Ba$_3$Cr$_2$O$_6$. We found evidence for field-induced magnetic order between Hc1 = 12.52(2) T and Hc2 \sim 23.6 T, with the maximum transition temperature Tc \sim 2.7 K at H \sim 18 T. There are many qualitative features of the data suggesting that the transition at Hc1 corresponds to a Bose-Einstein condensation of triplons universality class. These include the apparent preservation of U(1) symmetry for applied fields below Hc1, a highly symmetric phase diagram, and an absence of any magnetization plateaus in the magnetic torque and force measurements.

\textsuperscript{1}We acknowledge support from NSERC and CIFAR at McMaster.

2:54PM D31.00003 Specific heat measurements in the novel frustrated quantum magnets SrHoO$_4$ and SrDy$_2$O$_4$, A. D. BIANCHI, B. PREVOST, U. de Montreal, QC, Montreal, Canada, N. KURITA, F. RONNING, R. MOVSHOVICH, T. W. KLIEMCZUK, LANL, Los Alamos, NM, USA, M. KENZELMANN, LDM, PSI, Villigen, Switzerland, R. J. CAVA, Princeton University, Princeton, NJ, USA — We investigated the specific heat of the novel geometrically frustrated quantum magnets SrHoO$_4$ and SrDy$_2$O$_4$ to determine the nature of their ground states. We present a study of the magnetic field dependence of specific heat $C_p(T, H)$ measured in a dilution refrigerator between 0.1 K and 4 K and a PPMS between 2 and 50 K for magnetic fields H between 0 and 9 T. We subtracted the phonon background $C_{\text{ph}}$ by using a temperature dependent Debye temperature determined from measurements on the non-magnetic structural analogue SrLu$_2$O$_4$. After this subtraction, in SrHoO$_4$ we observed a broad anomaly in the magnetic specific heat $C_{\text{mag}} = C_p - C_{\text{ph}}$ centered at 0.5 K in zero field. At high fields, we found a broad peak centered at 0.35 K which decreases with rising magnetic field. SrDy$_2$O$_4$ in zero field has a broad anomaly at 1.2 K. The peak broadens with increasing H and its amplitude decreases, and by 5 T it is completely suppressed. By 50 K, each ion in the Dy compound has recovered 21.5 J/mol K of its spin entropy, which is comparable to the entire spin entropy of a free Dy ion of $R \cdot \ln(2J + 1)$, whereas we observe only 11.1 J/mol K for SrHoO$_4$.

3:06PM D31.00004 The Interplay of Quantum Criticality and Frustration in Columbite\textsuperscript{1}, RIBHU KAUL, Station Q, UCSB, SUNGBIN LEE, Department of Physics, UCSB, LEON BALENTS, KITP, UCSB — CoNb$_2$O$_6$ is a remarkable material. It can be modeled as a lattice of Ising chains coupled to each other in a frustrated anisotropic triangular lattice in the basal plane perpendicular to the chain direction. Applying a strong transverse field tunes the chains through a quantum phase transition into a paramagnetic phase. The interplay between two of the most interesting features of correlated quantum physics, quantum criticality and geometric frustration, produces a rich phase diagram which reflects the fundamental underlying quantum many-body physics. Using a variety of analytic and numerical techniques, we map out the phase diagram of this material in both transverse and longitudinal fields and provide a comparison with experiment.

\textsuperscript{1}This research was supported in part by Microsoft Corporation.

3:18PM D31.00005 Quantum phase transitions of the asymmetric three-leg spin tube, TORU SAKAI, JAEA/SPring-8, University of Hyogo, JST TRIP, MASAHIRO SATO, RIKEN, KOUCHI OKUNISHI, Niigata University, YUICHI OTSUKA, University of Hyogo, KIYOMI OKAMOTO, Tokyo Institute of Technology, CHIGAK ITOI, Nihon University — We investigate quantum phase transitions of the S=1/2 three-leg antiferromagnetic spin tube with asymmetric inter-chain (rung) exchange interactions. On the basis of the electron tube system, we propose a useful effective theory to give the global phase diagram of the asymmetric spin tube. In addition, using other effective theories we raise the reliability of the phase diagram. The density-matrix renormalization-group and the numerical diagonalization analyzes show that the finite spin gap appears in a narrow region around the rung-symmetric line. In contrast to a recent paper by Nishimoto and Arikawa \cite{1}. The numerical calculations indicate that this global phase diagram obtained by use of the effective theories is qualitatively correct. In the gapless phase on the phase diagram, the numerical data are fitted by a finite-size scaling in the $c=1$ conformal field theory. We argue that all the phase transitions between the gapful and gapless phases belong to the Berezinskii-Kosterlitz-Thouless universality class \cite{2}.

\begin{thebibliography}{1}
\end{thebibliography}

3:30PM D31.00006 Critical behavior study of antiferromagnetism in isostructural La$_2$CuO$_{4+\delta}$ and La$_2$NiO$_{4+\delta}$, BENJAMIN WHITE, JOHN NEUMEIER, Montana State University, A. ERB, Walther Meissner Institute — Neutron diffraction \cite{1} and nuclear quadruple resonance \cite{2} experiments coupled with theory calculations provide substantial evidence to support the widely-accepted belief that the two-dimensional Heisenberg model describes the antiferromagnetic interactions in La$_2$CuO$_4$ ($S = 1/2$) and La$_2$NiO$_4$ ($S = 1$). The heat capacity critical exponent $\alpha$, which could provide further evidence in these two compounds because of the weak nature of the anomalies at $T_N$. We present heat capacity and high-resolution thermal expansion measurements of La$_2$CuO$_4$ and La$_2$NiO$_4$ single crystals, grown by the floating-zone method, and an analysis of $\alpha$ within the context of predicted values for a variety of universality classes. This material is based upon work supported by the NSF (DMR-0504769) and US DOE Office of Basic Energy Sciences (DE-FG-06ER46260) \cite{1}.\cite{2} Y. Endoh et al., PRB 37, 7443 (1988); G. Aeppli and D.J. Buttrey, PRL 61, 203 (1988).

\begin{thebibliography}{2}
\bibitem{1} V. Enzehl et al., PRB 55, 3734 (1997).
\bibitem{2} T. Kyomen et al., PRB 60, 14841 (1999); K. Sun et al., PRB 43, 239 (1991).
\end{thebibliography}
3:42PM D31.00007 Physics of the spin gap in the $S = 1/2$ Heisenberg antiferromagnet on kagome$^1$, OLEG TCHERNYSHYOV$^2$, Johns Hopkins University — A combination of low spin and strong frustration makes the $S = 1/2$ Heisenberg antiferromagnet on kagome a likely candidate for an unusual ground state and elementary excitations. Exact-diagonalization studies$^1$ on finite clusters point to a lack of magnetic order in the ground state and to an energy gap of order $1/20$ for $S = 1$ excitations. The exact nature of the ground state and elementary excitations remains a subject of vigorous debate. Among the proposed ground states are chiral$^2$ and non-chiral$^3$ spin liquids and a valence-bond crystal (VBC)$^4-5$; spin excitations range from deconfined spinons with a Bose$^6$ or Fermi statistics$^2-3$ to magnons$^7$. We show that the system behaves as a collection of spinons, quasiparticles with $S = 1/2$ and Fermi statistics, whose motion disturbs valence-bond order. Attraction between spinons, mediated by exchange, binds them into small, massive pairs of $S = 0$ with a binding energy of $0.06 J$.$^8$ The pair formation strongly suppresses the motion of individual spinons and makes the survival of the Singh-Huse VBC plausible. A spin excitation amounts to breaking up a pair into two (nearly) free spinons with $S = 1$. The survival of the VBC is expected to lead to spinon confinement; however, small energy differences between various valence-bond configurations would make the confinement length large.

1Supported in part by DOE Grant DE-FG02-08ER46544.


1Supported in part by DOE Grant DE-FG02-08ER46544.

4:30PM D31.00009 ABSTRACT WITHDRAWN —

4:42PM D31.00010 Order and Disorder in AKLT Antiferromagnets in Three Dimensions$^1$, SIDDHARTH PARAMESWARAN, S.L. SONDHI, Princeton University, DANIEL AROVAS, UC San Diego — The models constructed by Affleck, Kennedy, Lieb, and Tasaki (PRL 58, 799 (1987)) describe a family of quantum antiferromagnets on arbitrary lattices, where the local spin $S$ is an integer multiple $M$ of half the lattice coordination number. The equal time quantum correlations in their ground states may be computed as finite temperature correlations of a classical O($3$) model on the same lattice, where the temperature is given by $T = 1/M$. In dimensions $d = 1$ and $d = 2$ this mapping implies that all AKLT states are quantum disordered. We consider the $d = 3$ case where the nature of the AKLT states is now a question of detail depending upon the choice of lattice and spin; for sufficiently large $S$ some form of Néel order is almost inevitable. On the unfrustrated cubic lattice, we find that all AKLT states are ordered while for the unfrustrated diamond lattice the minimal $S = 2$ state is disordered while all other states are ordered. On the frustrated pyrochlore lattice, we find (conservatively) that several states starting with the minimal $S = 3$ state are disordered. These are a significant addition to the catalog of magnetic Hamiltonians in $d = 3$ with ground states known to lack order on account of strong quantum fluctuations.

1Work supported in part by NSF Grant DMR0213706 (SLS).

4:54PM D31.00011 Global phase diagrams of frustrated quantum antiferromagnets in two dimensions: doubled Chern-Simons theory, CENKE XU, SUBIR SACHDEV, Harvard University — We present a general approach to understanding the quantum phases and phase transitions of quantum antiferromagnets in two spatial dimensions. We begin with the simplest spin liquid state, the $Z_2$ spin liquid, whose elementary excitations are spinons and visons, carrying $Z_2$ electric and magnetic charges respectively. Their dynamics are expressed in terms of a doubled U(1) Chern-Simons theory, which correctly captures the “topological” order of the $Z_2$ spin liquid state. We show that the same theory also yields a description of the variety of ordered phases obtained when one or more of the elementary excitations condense. Field theories for the transitions and multicritical points between these phases are obtained. We also survey experimental results on antiferromagnets on the anisotropic triangular lattice, and make connections between their phase diagrams and our results.

5:06PM D31.00012 Stability of the U(1) spin liquid with spinon Fermi surface in 2+1 dimensions$^1$, SUNG-SIK LEE, McMaster University — We study non-perturbative stability of a 2+1 dimensional critical spin liquid state, the U(1) spin liquid with a spinon Fermi surface. By mapping the spinon Fermi surface into an infinite set of 1+1 dimensional chiral fermions, we show that an instanton has an infinite scaling dimension for any nonzero N, where N is the number of spinon flavors. Therefore, the spin liquid state can be stable against confinement in physical systems, such as spin 1/2 magnets on the triangular lattice.

1This work was supported by NSERC.
5:18PM D31.00013 Finite-size scaling of string order parameters characterizing the Haldane phase. HIROSHI UEDA, Graduate School of Engineering Science, Osaka University, HIROKI NAKANO, Graduate School of Material Science, University of Hyogo, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University. We have developed a numerical procedure to clarify the critical behavior near a quantum phase transition by analyzing a multi-point correlation function characterizing the ground state. The procedure focuses on the gradient of the inverse-system-size dependence of the correlation function on a logarithmic plot. It requires only the correlation functions of several finite sizes under the same condition as a candidate for the long-range order. We apply the analysis to the string order parameter of the $S = 1/2$ XXZ chain with uniaxial single-ion anisotropy obtained by the density matrix renormalization group method. The present analysis gives precise estimates of transition points and critical exponents, $\nu$ and $\eta$, in Ising transitions, Gaussian transitions, and Berezinskii-Kosterlitz-Thouless transitions. Consistent results with those obtained from the analysis of the energy-level structure. This method will contribute much for a direct observation of quantum phase transitions.

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D32 GMAG DMP: Focus Session: Spin Dependent Physics in Organic Materials and Graphene 336

2:30PM D32.00001 Magnetism by nonmagnetic defects in a 2D BN sheet: ab initio studies. CHRISTOPHER MALEC, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology. Few layer graphene as well as thin graphite samples are measured by magnetic resonance (EPR) experiments (Eastern Washington University, JOHN SCHLUETER, Argonne National Laboratory). Latest results will be discussed.

2:42PM D32.00002 Magnetoresistance in hydrogen-doped graphene nanoribbons. F. MUNOZ-ROJAS, Universidad de Alicante, D. SORIANO, J. FERNANDEZ-ROSSIER, J. J. PALACIOS. Recent works have focused on hydrogen-doped graphene, both in the diluted and highly doped concentrations. It is known that a single hydrogen atom on top of a carbon atom in graphene has a magnetic moment. In the case of a low concentration of hydrogen dopants, it is believed that the ground state features local moments with zero total spin. Application of a strong enough magnetic field can spin polarize the system, in analogy with diluted magnetic semiconductors. In this work we study whether this spin order changes the resistance of the system. We study the relation between conductance and spin order for hydrogen-doped graphene armchair nanoribbons. We use both mean field Hubbard model and density functional theory calculations and compare results from both approaches. For the latter one, B3LYP hybrid functional is used. The conductance is calculated for the diluted limit. We use the Landauer formalism with the Green’s Function Approach for the conductance calculation. We find that the conductance in these systems is significantly affected by spin order. Thus, we predict magnetoresistance in graphene ribbons doped with Hydrogen.

2:54PM D32.00003 Spin dependent Transport in Thin Graphite and Few Layer Graphene. CHRISTOPHER MALEC, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology. Few layer graphene as well as thin graphite samples are measured by local and non-local spin injection techniques at 4.2 K. Both spin valve, and spin precession measurements are performed. Spins remain coherent over micron length scales. Latest results will be discussed.

3:06PM D32.00004 Magnetism and magnetic interactions in graphene and graphite. OLEG YAZYEV, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland. Magnetic materials and nanostructures based on carbon and other light elements provide a number of attractive opportunities for future information technologies such as spintronics and quantum information processing. In this talk, I review the first-principles studies of the magnetism induced by defects and edges in graphene and graphite. We show that in graphene the single-atom defects (e.g. vacancies and hydrogen chemisorption) induce the spin-polarized defect states in different defect configurations. We explain the recent experimental observations of high-temperature ferromagnetism in proton-irradiated graphite. Similarly, the zigzag edges of graphene are predicted to induce local magnetic moments which can serve as a base for novel spintronic devices. We address the question of the spin orientation stability length in this one-dimensional magnetic system and establish the limitations of the proposed spintronic devices [3]. Finally, I consider the hyperfine interactions (i.e. the magnetic interactions between the spins of electrons and nuclei) in carbon nanostructures and materials [4]. Possible approaches for achieving long electron spin decoherence times in graphene-based nanostructures are discussed.

3:42PM D32.00005 Determining the spatial and spin anisotropy of reduced-dimensionality Cu-based magnets using EPR, ultra-high-field magnetization and simulations. SUSAN COX, ROSS MCDONALD, JOHN SINGLETON, National High Magnetic Field Laboratory, PINAKI SENGUPTA, Los Alamos National Laboratory, PAUL GODDARD, STEPHEN BLUNDELL, Physics, University of Oxford, JANEZ BONCA, Physics, Ljubljana University, SAMIR EL SAWISH, Jozef Stefan Institute, JAMIE MANSON, Chemistry, Eastern Washington University, JOHN SCHLUETER, Argonne National Laboratory. Pulsed-field magnetization experiments (up to 85 T) and electron paramagnetic resonance (EPR) experiments (10 – 110 GHz) are reported on a family of organic Cu-based two-dimensional (2D) Heisenberg magnets. The low-$T$ $M(H)$ relationship is concave, with a sharp transition to a saturation value at a critical field $H_c$. Monte-Carlo simulations including a finite interlayer exchange energy quantitatively reproduce the data. Thus, one can obtain accurate values for both intra- and interlayer exchange energies. The EPR spectra show pronounced changes in effective $g$ factor, linewidth and zero-field intercept at temperatures, fields and frequencies of the same energy scale as the dominant exchange parameter. The EPR results are modeled using finite-cluster-size methods, and the data are well matched by an easy-plane spin anisotropy in the range 0.01 – 0.05. Thus, EPR measurements allow the spin orientation dependence of the exchange interaction to be determined.
3:54PM D32.00006 Fermomagnetic transition coupled to magnetoelastic interactions1. J.L. MUSELDT, L.I. VERSGARA, T.V. BRINZARIL, University of Tennessee, L.C. TUNG, Y.J. WANG, NHMFL, J.A. SCHLUETER, Argonne, J.L. MANSON, Eastern Washington, UNIVERSITY OF TENNESSEE TEAM, NHMFL TEAM, ARGONNE TEAM, EASTERN WASHINGTON TEAM — We investigate the magneto-infrared response of CuHF$_2$(pz)$_2$BF$_4$, a quasi-two-dimensional Heisenberg antiferromagnet, in order to probe the microscopic aspects of magnetoelastic coupling through the field-driven antiferromagnetic to ferromagnetic transition. The ferromagnetic transition is accompanied by substantial changes in the out-of-plane pyrazine ring distortion, suggesting a mechanism for explaining the soft magnetism of this system. The size of these field-induced distortions tracks the bulk magnetization, demonstrating that the ferromagnetic transition is coupled to magnetoelastic interactions in this material. We discuss these results in terms of local structural distortions and the effect on in-plane superexchange interactions.

We thank the Division of Materials Research at NSF for support of this work.

4:06PM D32.00007 Magnetic phase diagram of a 2D quantum Heisenberg antiferromagnetic compound Cu(pz)$_2$(ClO$_4$)$_2$, FAN XIAO, Clark University, NAT FORTUNE, Smith College, CHRISTOPHER LANDEE, MARK TURNBULL, Clark University — Cu(pz)$_2$(ClO$_4$)$_2$ is a 2D quantum Heisenberg antiferromagnet with an exchange strength of 17.5(5) K and a zero-field ordering temperature of 4.25 K. The ordering temperature has been found to be affected by an applied field. The phase diagram of Cu(pz)$_2$(ClO$_4$)$_2$ is determined by measuring the magnetization and the in-field specific heat. The behavior of the ordering temperature can be interpreted as a field induced 2D Heisenberg to 2D XY crossover.

4:18PM D32.00008 Gapped quantum spin-liquid state in a frustrated triangular magnet K-(BEDT-TTF)$_2$Cu$_3$(CN)$_3$, MINORU YAMASHITA, NORIHI TO NAKATA, Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan, YUI CHI KASAHARA, TAKAKIHO SASAKI, NAOKI YONEYAMA, NORIO KOYAYASHI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, SATOSHI FUJIMOTO, TAKASADA SHIBAUCHI, YUJI MATSUDA, Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan — Unveiling the nature of quantum-spin-liquid (QSL) states, quantum fluctuation-driven disordered ground states, has been a central challenge in condensed matter physics. Especially the nature of the low-lying spin excitations and the presence/absence of the “spin gap” have been of great interest. Recently, NMR measurements have shown that a QSL state is realized in n = (BEDT-TTF)$_2$Cu$_2$(CN)$_3$ with a nearly isotropic 2D triangular lattice structure. Here we report on our thermal-transport measurements in this compound down to 80 mK. We find that the QSL state has a full gap of ∼ 0.5 K (∼ 1/100) and the gap is hardly affected by magnetic fields up to 10 T [1], which sharply contradicts recent reports of heat capacity measurements reporting a finite γ-term. We will discuss some possibilities to explain this tiny spin gap in this present system. [1] M. Yamashita et al., Nature Physics (in press).

4:30PM D32.00009 Neutron scattering measurements of spin excitations in the spin ladder compound (pip)$_2$CuBr$_2$. A.T. SAVICI, C.L. BROHOLM, Dept. of Physics and Astronomy, Johns Hopkins Univ., Baltimore, MD, G.E. GRANROTH, S.E. NAGLER, NSDD, ORNL, Oak Ridge, TN, K.P. SCHMIDT, G.S. UHRIG, Technische Univ. Dortmund, Dortmund, Germany, D.M. PAJEROWSKI, M.W. MEISEL, Dept. of Physics, Univ. of Florida, Gainesville, FL, D.R. TALHAM, Dept. of Chemistry, Univ. of Florida, Gainesville, FL, C.M. BROWN, NIST Center for Neutron Research, Gaithersburg, MD — Recent theoretical and experimental work on S = 1/2 ladders has been inspired, in part, by the realization of a novel quantum spin liquid state. Bulk magnetization measurements indicate that (Cu$_2$H$_2$N)$_2$CuBr$_4$ (BPCB) is a two-leg spin ladder with stronger coupling along the rung (J$_H$) than along the leg direction (J$_L$) [1]. Here we report neutron spectroscopy measurements performed on a deuterated BPCB. We show that J$_H$ and J$_L$ are consistent with the previous measurements. No dispersion in the inter-ladder direction means that the ladders are magnetically isolated, likely due to frustrated inter-ladder exchange. We show that any diagonal exchange is < J$_H$/10, confirming that BPCB is an excellent realization of a S = 1/2 ladder in the strong coupling limit. [1] B.C. Watson et al., Phys.Rev.Lett. 86, 5168 (2001). *Work supported by NSF DMR-0603136, DMR-0701400, DMR-0543362, DMR-0454672, DOE DE-AC05-00OR22725, ESF and EuroHorcs.

4:42PM D32.00010 Neutron scattering measurements of the molecule-based magnets M[TCE]$_{n}$$(NCMe)$_{2}X$, ALEXANDER E. MIDGLEY, University of Missouri-Kansas City, KONSTANTIN POKHODNYA, C. OLSON, North Dakota State University, A.N. CARUSO, MICHAEL B. KRUGER, University of Missouri-Kansas City — M[TCE]$_{n}$$(M=V, Fe, Mn, Co, Ni; X=tetracyanoethylene) molecule-based magnets demonstrate high magnetic ordering due to a strong antiferromagnetic interaction between the unpaired d- and p-electrons of the metal ions and the ligands; however, the type of bonding involved in the superexchange mechanism remains unclear. The Raman active C-C vibration depends solely upon the degree of charge transfer from the metal ion to the π-active C=C vibration. Raman spectra of the M[TCE]$_{n}$$(M=Fe, Mn, Ni; X=FeCl$_3$, SbF$_6$) molecule-based magnets were collected in a diamond anvil cell at pressures up to 36 kbar. The observed pressure-induced strengthening of the ν(CC) and ν(CN) Raman modes provides a clearer picture of the type and degree of backbending, which will ultimately help build a model of how superexchange is occurring in these systems.

5:04PM D32.00011 Bonding, Backbonding and Spin-Polarized Molecular Orbitals: Basis for Magnetism and Semiconducting Transport in V[TCE]$_{2}X$, JEFFREY KORTRIGHT, Lawrence Berkeley National Laboratory, DEREK LINCOLN, RUTH SHIMA EDELSTEIN, ARTHUR EPESTEIN, The Ohio State University — V[TCE]$_{2}$ films exhibit magnetic order up to 400 K, magneto-resistance, and photo-induced magnetism. Yet the spin-polarized interactions between the TM and molecular species underlying these properties have remained elusive, in part because of its structural disorder. Using element-specific x-ray absorption spectroscopy (XAS) and magnetic circular dichroism (MCD) at the V L edges, and the C and N K edges we have gained new insight into these mechanisms [1]. We find evidence for covalent bonding between the V $\epsilon$L and TCE σ MO states, and a bridging interaction between V $\chi$MO and TCE π MO states, consistent with a generalized bonding/backbending model with V octahedrally coordinated by N in σ-bridging positions between TCE radical anions. C and N XAS and MCD reveal spin-polarized splitting of the former LUMO of neutral TCE, indicating that a direct exchange interaction underlies these properties. This indicates an active role of TCE* in the magnetic properties of extended V[TCE]$_{2}$ and related systems, which is distinctly different from superexchange models generally used to describe magnetic Prussian blue analogs. [1] Phys. Rev. Lett. 100, 257204 (2008).

Supported by DOE/BES and AFOSR.

5:06PM D32.00012 XPS and UV/Vis MCD studies of M[TCE] organic-based magnets, SAAD JANJUA, University of Missouri Kansas City, KONSTANTIN POKHODNYA, Center for Nanoscale Science and Engineering, Fargo,ND, MARCUS DRIVER, ANTHONY CARUSO, University of Missouri Kansas City, CARUSO'S RESEARCH GROUP TEAM — M[TCE]$_{n}$$(M=V, Fe, Mn, Ni; TCE = tetracyanoethylene) organic-based magnets provide a systematic means of studying magnetic superexchange by varying the 3d $\epsilon$L and $\epsilon$H filling. X-ray photoemission binding energy spectra of core electrons C (1s), N (1s) and M (3p) were used to study valency and bond type, giving a correlation between binding energy and transition temperature. UV/Vis Magnetic Circular Dischroism studies were conducted to investigate lowest unoccupied state and onsite Coulomb repulsion for both M 3d and TCE π* orbital. This talk will focus on providing empirical evidence of the near Fermi edge spin polarized electron structure in the context of magnetic exchange.
2:30PM D33.00001 Giant nonlinear electron-lattice interaction in cuprate superconductors, and origin of the pseudogap1, DEENNIS NEVINS, IBM T.J. Watson Research Center — The pseudogap is a key property of the cuprate superconductors, whose understanding should illuminate the pairing mechanism. Recent data support a close connection between the pseudogap and an oxygen-driven C4 symmetry breaking within the CuO2 plane unit cell. Using ab initio Molecular Dynamics, we show the existence of a strong nonlinear electron-oxygen vibrator coupling in two cuprates. In a mean field approach applied to this coupling, we derive a C4 splitting/pseudogap phase diagram in agreement with experiment — providing an explanation for the pseudogap phenomenon from first principles. The implications for superconductivity, Fermi surface arcing, and other properties are discussed.

2:42PM D33.00002 An explanation of the dichotomy between Fermi arcs and Fermi pockets in underdoped high-\(T_c\) superconductors1, XUN JIA, SUDIP CHAKRAVARTY, University of California at Los Angeles — We have numerically computed the spectral function \(A(\vec{k},\omega)\) of an underdoped cuprate superconductor for the \(d\)-density wave state subject to a long range correlated disorder. The intensity of the spectral function is significantly reduced for the electron pockets for an intermediate range of correlation length, but the Fermi arcs remain quite intact. This result provides one possible explanation as to why the electron pockets are not observed in angle resolved photoemission experiments. A calculation of Shubnikov-de Haas (SdH) oscillations using a real space transfer matrix method shows that two main frequencies are still present in the presence of a moderate amount of white noise disorder. The SdH oscillations in other relevant broken symmetry states are also computed.

2:54PM D33.00003 Quantum oscillations in a highly renormalized Fermi liquid model of Fermi pockets in underdoped cuprates1, TUDOR STANESCU, VICTOR GALITSKI, University of Maryland, DENNIS DREW, CNAM, University of Maryland — Motivated by the recent experimental observation of quantum oscillations in the underdoped cuprates, which suggest the existence of small electron pockets characterized by a relatively large cyclotron mass, we address two basic questions: 1) How can one explain the relatively large cyclotron effective mass observed experimentally and its relation with the effective Hall mass? 2) Why the electron pockets are not seen in ARPES experiments? We propose an explanation based on a model of a highly renormalized Fermi liquid characterized by a reconstructed Fermi surface and strongly momentum-dependent quasiparticle properties. We find that the cyclotron mass is enhanced by a factor \(<1/Z>\), while the effective Hall mass is proportional to \(<Z>/<Z^2>\), where \(<...>\) implies an averaging over the Fermi surface. If the \(Z\)-factor becomes small in some part of the Fermi surface, the cyclotron mass is enhanced sharply while the infrared Hall mass may remain small.

3:06PM D33.00004 Superconductivity near structural phase transition: the case of NbN1, SIMON BLACKBURN, MICHEL CÔTÉ, Département de physique, Regroupement québécois des matériaux de pointe (RQMP), Université de Montréal, CANADA, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, University of California at Berkeley and Materials Sciences Division of Lawrence Berkeley National Laboratory — Using density functional theory within the local density approximation we report the study of the electron-phonon coupling in NbC1-xN x crystals in the rocksalt structure. The Fermi surface of the system allows important nesting. The associated Kohn’s anomaly greatly increases the electron-phonon coupling and induces a structural instability when the electronic density of states reaches a critical value. Our results reproduce the observed rise in \(T_c\) from 11.2 K to 17.3 K as the nitrogen doping is increased. To further understand the important effect of the structural instability to the superconducting temperature, we model the Eliashberg spectral function with two contributions, one for the unstable phonons and the other for the unaffected phonons. Using the McMillan formula, we can predict the evolution of \(T_c\) within this simple model that reproduces well our \(ab\) initio results and the experimental data.

3:18PM D33.00005 Competition between antiferromagnetism and superconductivity, electron-hole doping asymmetry and “Fermi Surface” topology in cuprates1, SANDEEP PATHAK, Indian Institute of Science, VIJAY SHENOY, IISC Bangalore and Ohio State, NANDINI TRIVEDI, MOHIT RANDERIA, The Ohio State University — We study the asymmetry between electron and hole doping in a 2D Mott insulator, and the resulting competition between antiferromagnetism (AF) and \(d\)-wave superconductivity (SC), using variational Monte Carlo for projected wave functions. We find that key features of the \(T_c\) vs \(d\) phase diagram, such as critical doping for SC-AF coexistence and the maximum value of the \(SC\) order parameter, are determined by a single parameter \(\eta\) which characterizes the topology of the “Fermi surface” at half filling defined by the bare tight-binding parameters. Our results give insight into why AF wins for electron doping, while SC is dominant on the hole doped side. We also suggest using band structure engineering to control the \(\eta\) parameter for enhancing SC.

3:30PM D33.00006 Density Matrix Renormalization Group Study of a Dynamic Hubbard Model, a Comparative Study1, FATIH DOGAN, University of Alberta, Edmonton, AB, Canada, FRANK MARISGLIO, University of Alberta — A one-dimensional model of holes locally coupled to pseudo spin degrees of freedom is studied using density matrix renormalization group. The model used in this talk is one in the family of dynamic Hubbard models. We look at density-density correlations, and frequency dependent functions to see existence and nature of the attraction of the holes in an electron-hole asymmetric system.

3:42PM D33.00007 ABSTRACT WITHDRAWN —
3:54PM D33.00008 Valence bond glassy order and the pseudogap phase in underdoped high Tc cuprates. LIANG, REN, ZIQIANG WANG, Boston college — Different origins of the pseudogap phenomena in underdoped high Tc cuprate have been proposed over the years, but a consistent theory has been challenging. We argue that the low-energy fluctuations of the valence bond, originating from the superexchange interaction, are pinned by the doping induced electronic disorder to give rise to a valence bond glass (VBG) pseudogap phase. Using an extended t-J model within the Gutzwiller approximation, we show that the normal state VBG phase exhibits a genuine Fermi arc and a V-shaped average density of state at low energies. In the superconducting phase below Tc, the VBG can coexist and compete with an inhomogeneous d-wave superconductor, leading to the two-gap phenomena. We discuss the evolution of the local and momentum-space spectroscopy with doping and temperature, which capture the salient properties of the pseudogap phenomena and electronic disorder observed by recent ARPES and STM experiments.

4:06PM D33.00009 On stability of odd-frequency superconducting state. DMITRY SOLENOV, IVAR MARTIN, DAMITRY MOZRYSKY, Theoretical Division, Los Alamos National Laboratory — Odd-frequency pairing mechanism has been investigated for several decades. Nevertheless the properties of such superconducting phase as well as its thermodynamic stability have remained unclear. In particular it has been argued by numerous authors that the odd-frequency state is thermodynamically unstable, has an unphysical Meissner effect (at least within the mean-field approximation), and therefore can not exist as a homogeneous phase in equilibrium physical systems. We argue that such a conclusion is incorrect because it relies on an inappropriate assumption that the odd-frequency superconductor can be described by an effective Hamiltonian that breaks the U(1) symmetry. We show that the odd-frequency state can be appropriately formulated within the functional integral representation by using the effective action to describe such a superconducting state within the mean field approximation. We find that the odd-frequency superconductor is thermodynamically stable and exhibits ordinary Meissner effect, and therefore, in principle, it can be realized in equilibrium solid state systems.

4:18PM D33.00010 Wave function for composite odd-frequency superconductors. HARI DADA, Los Alamos National Laboratory, ELIHU ABRAHAMS, Department of Physics and Astronomy, Rutgers University, DMITRY MOZRYSKY, Los Alamos National Laboratory, YUKIO TANAKA, Department of Applied Physics, Nagoya University, JAPAN, ALEXANDER BALATSKY, Los Alamos National Laboratory — Berezinskii proposed a new class of superconducting state that has an anomalous gap function that is odd function of frequency. Following initial work of Berezinskii there has been growing interest in properties of such superconductors. We propose a BCS-like wave function for an s-wave triplet odd-frequency superconductor. The wave function describes a condensate of spin-0 Cooper pair and spin-1 magnon, a composite order parameter. By minimizing a Hamiltonian, suggested earlier in Ref. [3] to study the odd-frequency superconductor, we derive the quasiparticle dispersions, the self-consistent gap equation, and the density of states. We show that the odd-frequency state is thermodynamically stable and exhibits ordinary Meissner effect, and therefore, in principle, it can be realized in equilibrium solid state systems.

4:30PM D33.00011 Ginzburg Landau Theory for Cuprate Superconductivity. TIRUPPATTUR RAMAKRISHNAH, Dept. of Physics, Indian Institute of Science, Bangalore 560012, Also Banaras Hindu University, Varanasi 221005, INDIA, SUMILAN BANERJEE, CHANDAN DASGUPTA, Dept. of Physics, Indian Institute of Science, Bangalore 560012, INDIA — We propose and develop the consequences of a theory of a cuprate is expressed as a functional of the complex nearest neighbour spin singlet bond pair order parameter $\Delta_{ij} \exp(i\phi_{ij})$, $F$ is a sum of two terms $\sum_{m,n}(a\Delta^2_m+b\Delta^2+n)$, and $F_1 = -\sum_{m,n} x m c \cos(\phi_{mn} - \phi_{ij});$ here $m$ is the site corresponding to $ij$ on the dual lattice (also square) and $m, n$ are nearest neighbours. The doping $x$ and temperature $T^*$ dependences of $a, b$ and $c$ are rationalized (eg, $a \propto x$ for small $x$). The pseudogap (due to incoherent bond pairs) and the parabolic $x$ dependence of $T_c$ (AF ordering of the 2d-XY spin $\Delta_{mn} \exp(i\phi_{mn})$ leading to d wave superconductivity) are described. The observed $C_1(T)$ behaviour is shown to be due to disorder parameter fluctuations. Detailed calculations of the vortex structure show a crossover from a Josephson like to a BCS like form with increasing doping, mirroring a similar change in superconductivity.

4:42PM D33.00012 Levitation and lateral forces between a small magnet and superconducting sphere and the stability of the magnet. H. AL-KHATEEB, M. ALQADI, F. ALZOUBI, B. ALBISS, M. HASAN, N. AYOUB, Department of Physics, Jordan University of Science & Technology — Using the dipole-dipole interaction model, we obtained analytical expressions for the levitation and lateral forces act on a small magnet for anti-symmetric magnet/spherical superconductor system. Breaking the symmetry of the system, allow us to study the lateral force which is important in the stability of the magnet above superconducting sphere in the Meissner state. Our formulas are written in terms of the radius of the superconductor as well as the height, the lateral displacement and the orientation of the magnetic moment of the magnet. We found that the levitation force is linearly dependent on a lateral displacement whereas the lateral force is independent of the lateral displacement. Moreover, the levitation and lateral forces are varying solinoidally with the polar and azimuthal angle of the orientation of the moment of the magnet. The stability of the magnet has been discussed for special orientations of the moment of the magnet.

4:54PM D33.00013 HTSC Measurements Explained by Defended Superconductivity Theory. JOHN JAMES, St. Louis University — Resonance between the superconducting gap and the low energy optical phonon mode creates a burst of coherent phonons which prevents the unstable superconducting state from collapsing. Surrounding lattice defects with charge states prevents interactions which would stop the coherent phonons from forming. This simple model of why $T_c$ is high can explain many other phenomena, such as; insufficient density of states and phonons which prevents the unstable superconducting state from collapsing. Surrounding lattice defects with charge states prevents interactions which would stop the coherent phonons from forming.

5:06PM D33.00014 A Dynamical Mean Field Study of the Three-Band Copper-Oxide Model. XIN WANG, Columbia University, LUCA DE' MEDICI, Rutgers University, CAPONE MASSIMO, Università di Roma La Sapienza, ANDREW J. MILLIS, Columbia University — We apply the dynamical mean field theory to study the three-band Copper-Oxide Model related to the High-Tc Cuprates. Both continuous-time quantum Monte Carlo and Exact Diagonalization impurity solvers are used. The spectral function, mass enhancement and optical conductivity in both paramagnetic and antiferromagnetic case are computed. We determine the contribution of antiferromagnetic order to the gap observed in the undoped material. We show that in the paramagnetic Mott insulating regime the quasiparticle mass enhancement is larger for hole than for electron-doped compounds, but an opposite trend in matrix elements means that a the optical conductivity in these two cases is comparable.

5:18PM D33.00015 Retarded vs instantaneous interactions in high-temperature superconductors. What is the glue?1.21 BUMSOO KYUNG, DAVID SENECHAL, A.-M.S. TREMBLAY, Université de Sherbrooke — In BCS theory, the phononic origin of the attraction that leads to Cooper pairs was confirmed by theoretical and experimental developments that clearly showed that the interaction was retarded and that the corresponding energy scales were associated with phonons. Using Cellular Dynamical Mean-Field Theory with exact diagonalization at $T = 0$, we identify retardation effects in pairing and associate the corresponding energy scales with the spectral function of short-range spin fluctuations. These fluctuations are clearly seen in neutron and optical spectroscopy probes. Since the pairs have vanishing wave function at zero distance, the energy scale $U$ is absent from the pair dynamics. That dynamics can be monitored by the anomalous spectral weight. The Heisenberg exchange $J$ is a characteristic energy scale of that spectral weight and it appears in a manner analogous to what is found in mean-field theories. However, the anomalous spectral weight has additional structure caused by retardation.

1NSERC, CRC, CFI, CIFAR.

Monday, March 16, 2009 2:30PM - 5:30PM – Session D34 DCMP: Superconductivity: Josephson Effects 404

2:30PM D34.00001 Temperature and Field Dependence of the Emission of Terahertz Waves from Intrinsic Josephson Junctions1.2 YOSHIHIKO NONOMURA, Computational Materials Science Center, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan — We have recently succeeded in extracting coherent cw THz-radiation from intrinsic Josephson junctions in BSCCO [Science 318, 1291, (2007)]. An electromagnetic cavity resonance inside the sample generates a coherent state in which a large number of junctions are synchronized to oscillate in phase resulting in emission powers of up to 5 µW at frequencies up to 0.85 THz. The emission displays a non-monotonic temperature dependence with a sample dependent sharp maximum in the range of 25 to 45 K which we attribute to the interplay of self-heating effects and re-trapping of intrinsic junctions. Application of magnetic fields of less than 100 Oe parallel to the CuO planes as well as perpendicular leads to the rapid suppression of the emission.

2:42PM D34.00002 Spin-Josephson effect in antiferromagnetic tunnel junctions1.2 DOMINIQUE CHASSE, A.-M.S. TREMBLAY, Université de Sherbrooke — In the Josephson effect, coherent Cooper pair tunneling is driven by the phase difference between the superconducting order parameters on opposite sides of the junction. By analogy, differences in order parameters across a junction should lead to coherent tunneling of the condensed objects that exist in the broken symmetry state. To exhibit the generality of this phenomenon and make predictions from a realistic model, we study the case of a tunnel junction between two itinerant antiferromagnets. At the mean-field level, we find an equilibrium current of the staggered magnetization through the junction that is proportional the normal state conductance and to $S_{x}$ x $S_{y}$ where $S_{x}$ and $S_{y}$ are the staggered magnetizations on either sides. Microscopically, this effect comes from coherent tunneling of spin-one charge-zero particle-hole pairs that have a net wave vector equal to the antiphase difference between one and zero spin projection along the direction of the order parameter. We explain similarities and differences with the standard DC and AC Josephson effects.

1CRSNG, CRC, CIFAR

2:54PM D34.00003 Angular dependence of the radiation power of a Josephson STAR-emitter1.2, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — We calculate the angular dependence of the power of stimulated terahertz amplified radiation (STAR) emitted from a dc voltage applied across a stack of intrinsic Josephson junctions. During coherent emission, we assume a spatially uniform ac Josephson current density in the stack acts as a surface electric current density antenna source, and the cavity features of the stack are contained in a magnetic surface current density source. A superconducting substrate acts as a perfect magnetic conductor with $H_{c1,ac}$ = 0 on its surface. The combined results agree very well with recent experimental observations. Existing Bi$_{2}$Sr$_{2}$CaCu$_{2}$O$_{8+δ}$ crystals atop perfect electric conductors could have Josephson STAR-emitter power in excess of 5 mW, acceptable for many device applications.

1supported by JST, CREST, MANA, CTC, and MEXT.

3:06PM D34.00004 Surface effects in THz wave emission from intrinsic Josephson junctions1.2 YOSHIIKO NONOMURA, Computational Materials Science Center, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan — Recently THz wave emission from intrinsic Josephson junctions without external fields [1] was observed experimentally. As possible states to characterize this emission, the McCumber-like state with little spatial dependence of electric fields (for the surface impedance $Z_{c}$ = 1) [2] and novel phase-kink state (for large and complex $Z$) [3] have been proposed. In the present study [4] it is numerically shown that both states are stationary and that the dynamical phase transition between these two states occurs as $Z_{c}$ is varied. The McCumber-like state is stable for low current and small $Z_{c}$. For higher current, the phase-kink state accompanied with symmetry breaking along the $c$ axis is stable even for $Z_{c}$ = 1, though strong emission in the vicinity of cavity resonance points only takes place for larger $Z_{c}$. Value of $Z_{c}$ is optimized for the strongest emission, and effect of surface roughness will also be discussed. [1] L. Ozyuzer et al., Science 318, 1291 (2007); [2] Kadowaki et al., Physica C 468, 634 (2008); [3] Y. Nonomura, arXiv:0810.3756.

3:18PM D34.00005 All-MgB$_{2}$ sandwich-type Josephson junctions with MgO barrier1.2 KE CHEN, CHENGGANG ZHUANG, QI LI, Department of Physics, Penn State University, University Park, PA 16802, YE ZHU, PAUL VOYLES, Department of Materials Science and Engineering, University of Wisconsin, Madison, WI 53706, X. X. XI, Department of Physics and Department of Materials Science and Engineering, Penn State University, University Park, PA 16802 — Reproducible all-MgB$_{2}$ Josephson junctions have been made to meet the expectation for superconducting electronics that can work at above 20 K. The sandwich-type junctions were fabricated using MgB$_{2}$ electrodes grown by hybrid physical-chemical vapor deposition and MgO barrier deposited by RF magnetron sputtering. The $I-V$ characteristics show tunneling behavior with a small resistive shunt. The $I_{c}R_{n,prod}$ product is 2.1 and 0.7 mV at 4.2 and 20 K, respectively, with temperature dependence following the theory qualitatively. The junctions exhibit good Fraunhofer pattern and Shapiro steps under applied magnetic field and microwave radiation, respectively. The $J_{c}$ of the junction varies exponentially with the barrier thickness, from 100 to 0.01 A/cm$^{2}$. Transmission electron microscopy reveals both MgB$_{2}$ layers are epitaxially grown with $c$-axis parallel to the SiC (0001) substrate normal. With the same chip $J_{c}$ speed less than 10%, this junction technology has the potential for MgB$_{2}$ circuits.

1Supported by ONR and NSF.
3:30PM D34.00006 Direct observation of THz radiation from cylindrical structure of intrinsic Josephson junction system of Bi2212, M. TSUJIMOTO, T. YAMAMOTO, H. MINAMI, K. KADOWAKI, M. TACHIKI, University of Tsukuba, U. WELP, W. KWOK, Argonne National Laboratory — Intense terahertz (THz) radiation was observed from a single crystalline high-Tc superconductor Bi2Sr2CaCu2O8+δ (Bi2212) system1–2. We have performed various experiments on THz radiation with Bi2212 rectangular mesa structure fabricated by Argon-ion-milling and photolithography technique with changing the sample parameters. In this work, we report new experimental results obtained with samples which have a cylindrical structure fabricated by focused ion beam milling. The intense emission of electromagnetic radiation can be obtained in the return branch only. The frequency is directly measured by FT-IR spectrometer to be \( f = 0.474 \) THz in this particular sample of diameter with 90 \( \mu \)m. This frequency value is in good agreement with the fundamental cavity resonance mode frequency. 1) L. Ozyuzer et al., Science 318 (2007) 1291 2) K. Kadowaki et al., Physica C 468 (2008) 634-639

3:42PM D34.00007 Sin(2\( \phi \)) component in the current-phase relation of SFS Josephson junctions near the 0-\( \pi \) transition, M. A. STOUTIMORE, Department of Physics, University of Illinois at Urbana-Champaign, A. YU. RUSANOV, V.A. OBOZNOV, V.V. BOLGINOV, A.N. ROSSOLENKO, V.V. RYAZANOV, Laboratory of Superconductivity, Institute of Solid State Physics, Russian Academy of Sciences, D.J. VAN HARLINGEN, Department of Physics, University of Illinois at Urbana-Champaign — We directly determined the Josephson current-phase relation (CPR) of superconductor-ferromagnet-superconductor (SFS) junctions by rf-SQUID interferometry, and corroborated it with measurements of the critical current as a function of temperature and magnetic field and rf-induced Shapiro steps in the current-voltage characteristics. Our Nb-Cu41Ni53:Nb trilayer junctions, with 2\( \times \mu \)m\(^2\) area and 7nm CuNi thickness, show a transition with temperature from the usual Josephson 0-junction state to a \( \pi \)-junction state, defined by a phase difference of \( \pi \) in the ground state, at temperatures between 1.5K and 3.5K. Near the transition, we observe second harmonics in the CPR, deviations from the usual Fraunhofer diffraction pattern and half-integer Shapiro steps, all consistent with a sin(2\( \phi \)) component in the CPR.

3:54PM D34.00008 Josephson interferometry evidence for order parameter with anisotropic and possibly complex phase in UPt3, J. B. KYCIA, J. P. DAVIS, WILLIAM HALPERIN, Northwestern University — The unconventional superconductor UPt3 exhibits many interesting properties. Among the most exciting is that it has two superconducting transitions, believed to arise from different degenerate order parameters, at least one of which breaks time-reversal symmetry. The nature of the order parameter in each of these phases and the crossover between them is still not fully understood. We have fabricated Josephson junctions on various faces of high quality single crystals of UPt3. Measuring the magnetic field dependence of the critical current through these junctions produces patterns that reveal the intrinsic phase differences and underlying symmetry of the order parameter. Our results point to an order parameter with anisotropic and possibly complex phase that extends throughout the entire crystal. This is in contrast with our work on Sr2RuO4, which also breaks time-reversal symmetry but exhibits a distribution of dynamic chiral order parameter domains.

4:06PM D34.00009 Interactions between Josephson Junction Metamaterials and Evanescent Waves, LAURA ADAMS, Center for Nanophysics and Advanced Materials, Physics Department, University of Maryland, College Park, MD 20742, STEVEN ANLAGE, Center for Nanophysics and Advanced Materials, Physics Department, University of Maryland, College Park, MD 20742 — Amplification of evanescent waves is an exciting, yet controversial application of negative index of refraction metamaterials in pursuit of creating a "perfect lens". We will describe evanescent wave amplification experiments using lossless metamaterials, i.e. arrays of Josephson junctions (JJ). The effects of input power, temperature, and dc magnetic field on JJ arrays below the cutoff frequency of a waveguide have been investigated. At low temperatures a pronounced, tunable microwave resonance emerges in transmission. This resonance has been systematically studied in terms of its transmission and reflection coefficients. In the regime between -45 and -25 dBm, we observe a non-hysteretic emission of microwave photons that reverberate at the same frequency. Amplification of these photons (parametric amplification) will also be described. This work was supported by the Intelligence Community Postdoctoral Fellowship program.

4:18PM D34.00010 Direct test of pairing fluctuations in the pseudogap phase of an underdoped cuprate, JEROME LESUEUR, NICOLAS BERGAL, LPEM, MARCO APRILI, LPS, BRIGITTE LERIDON, LPEM, GIANCARLO FAINI, LPN, JEAN-PIERRE CONTOUR, Thales-CNRS — In underdoped cuprates, many experiments have provided evidence for the presence of a gap-like structure in the electronic excitations spectrum, in a region above the critical temperature and below a characteristic temperature \( T^* \). The origin of this so-called pseudogap is still hardly debated and the answer to this question turns out to be essential for the understanding of high-Tc superconductivity. One doesn’t know if the pseudogap is related to superconductivity or to an order in competition. In the former case, it has been suggested that superconducting pairing fluctuations may be responsible for the partial suppression of electronic excitations. This remains to be tested experimentally, but most of the probes used to investigate the pseudogap are not sensitive to pairs and therefore cannot provide such a test. Here, we report for the first time on a direct test of pairing fluctuations in the pseudogap regime using a Josephson-like experiment. Our results shows that fluctuations survive only in a restricted range of temperature close to \( T_c \) (\( T-T_c<15K \)), and therefore cannot be responsible for the opening of the pseudogap at high temperature. Nature Physics 4, 608 - 611 (2008)

4:30PM D34.00011 ABSTRACT WITHDRAWN

4:42PM D34.00012 Underdamped fluxon diffusion in a Josephson junction parallel array, KENNETH SEGALL, Colgate University, JUAN MAZO, University of Zaragoza, ADAM DIOGUARDI, UC Davis, NIKHIL FERNANDES, Colgate University — We present experimental measurements and numerical simulations on the dynamics of fluxons in a parallel array of Josephson junctions. Fluxons trapped in a parallel array of Josephson junctions upon cooldown experience a periodic potential determined by the junction critical currents and the cell inductances. As shown in two recent papers [1,2], under certain conditions fluxons can move through the array in a series of noise-induced phase slips. This leads to a low-voltage diffusion branch in the current-voltage characteristics, similar to that in underdamped phase diffusion for a single junction. Unlike underdamped phase diffusion, however, this fluxon diffusion does not need frequency-dependent damping to occur. We demonstrate the existence of this state by direct measurements of the current-voltage characteristics and measurements of the switching current distribution of the array. 1. J.J. Mazo et al. Phys. Rev. B78, 174510 (2008) 2. K. Segall et al. http://arXiv.org/abs/0807.2978, to appear in J. Low Temp. Phys.
4:54PM D34.00013 A tunable Josephson current in a Rashba Ring by Aharonov-Casher Phase
XIN LIU, MARIO F. BORUNDA, XIONG-JUN LIU, JAIRO SINOVÁ1, Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA. JAIRO SINOVÁ’S GROUP AT TAMU TEAM — We study the interference effect induced by the Aharonov-Casher (A-C) phase on the transport between an asymmetrically confined two-dimensional electron ring system and the superconducting leads of a Josephson junction. The Josephson phase and the Andreev levels are studied both analytically and numerically. Our results also predict oscillations in the Josephson current due to the A-C phase in the ring that can be tuned electrically via the spin-orbit (SO) interaction. Based on these oscillations, we propose a novel mechanism to observe the A-C phase in mesoscopic rings with gate tunable SO interaction attached to superconducting leads using the Josephson current oscillations. An applicable method to control the Josephson current by a tunable gate voltage can be realized due to these phenomena.

1Principal Investigator

5:06PM D34.00014 Enhanced thermal activation of a superconductor-normal metal quantum interference device1, JIAN WEI, PAUL CADDEN-ZIMANSKY2, Northwestern University, VENKAT CHANDRASEKHAR — We measure the magnetoresistance and current-voltage characteristics (CVC) of a superconductor-normal metal quantum interference device in the form of a mesoscopic normal-metal loop in contact with two superconducting electrodes. Below the transition temperature of the superconducting leads, sharp switching from the zero-resistance state to a finite-resistance state is observed at half-flux quantum. The CVC in the finite-resistance state can be described by the Ambegaokar-Halperin (AH) theory of the effect of thermal fluctuations in Josephson junctions, but here this effect of thermal fluctuations is greatly enhanced. The CVC in the zero-resistance state can be described by the Langer-Ambegaokar-McCumber-Halperin theory of thermally activated phase slips in one dimensional superconductors, but also with enhanced phase slipping rates, or equivalently, lowered energy barriers.

1This was funded by the NSF through grant DMR-0604601.

5:18PM D34.00015 Static and dynamic effects in Superconducting/Normal metal/Superconducting long junctions, FRANCESCA CHIODI, BERTRAND REULET, HÉLENE BOUCHIAT, Laboratoire de Physique des Solides UMR 8502 — Université Paris-Sud, Bât 510 — 91405 Orsay cedex, LES NANOSTRUCTURES À LA NANOCONSEDE TEAM, PHYSIQUE MÉSOCOPICIE TEAM, J.C. CUEVAS-DEPARTEMENTO DE FISICA TEORICA DE LA MATERIA CONDENSADA-UNIVERSIDAD AUTONOMA DE MADRID COLLABORATION — We have studied four different Nb/Al long junctions at temperatures between 1.4 K and 4K (where the Al wire is still in the normal state). We have measured their low frequency current-voltage characteristics in the presence of an RF excitation (whose frequency varies from 100 kHz to 40 GHz). All the junctions show an important increase in critical current for frequencies above a threshold, which depends on the length of the normal wire. Is Thouless frequency playing a role? We have also studied the influence of geometry (narrow / square normal wire) on W/Au junctions. We have seen that the critical current/magnetic field curve changes from the well known Fraunhofer pattern (square wire) to a Gaussian dependence (narrow wire). We are interested in dynamic properties of SN junctions: inductively coupling a multilode LC resonator to an AC SQUID we hope to define the behaviour of Andreev bound states when excitation time becomes lower than the typical diffusion time.

Monday, March 16, 2009 2:30PM - 5:30PM —
Session D35 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors IV: General Experiment 408

2:30PM D35.00001 Iron Pnictide Superconductors: discovery and advances, HIDEO HOSONO, Tokyo Institute of Technology — Superconducting transition in a layered ZrCuSiAsS-type crystal was first reported for LaFePO in 2006 [1] and subsequently, a similar Tc was found for LaNiPO with the same crystal structure in 2007. However, Tc of these compounds reminded low (∼4K). On February 23, 2008, our paper reporting a layered compound in LaFeAsO1−xFex (x=0.1) exhibiting a superconducting critical temperature Tc (mid-point) = 26K was published [3]. In this presentation I talk the background of this discovery and the subsequent advance in materials. The following points have been clarified to date; (1) Iron-based superconductors reported are 4-types crystal structures, the 1111 [3], 122 [4], 111 [5], and 11 [6] type. All the high Tc iron-based superconductors contain a FeAs plane and the Fe3d orbitals dominate the Fermi-level. (2) The occurrence of a crystallographic transition accompanying anti-ferromagnetic to paramagnetic state in the parent compound is a requisite for a high Tc. (3) There exist a vast number of materials containing the Fe square lattice. (4) A partial substitution of Fe with other transition metal is possible without serious reduction of Tc. (4) A new insulating layer AEF (AE=Ca, Sr)was found to be effective in the 1111 phase [7]. (5) High pressure synthesis was effective to obtain the 1111 phases with higher Tc. (6) Epitaxial thin films exhibiting a Tc almost the same as that in the bulk were fabricated for CaFeAsO-Co[8]. Epitaxial thin films of LaFeAsO was recently reported as well [9].


3:06PM D35.00002 Materials and Physics in Pnictide Superconductors, HAI-HU WEN, IOP, CAS — Superconductivity in the pnictides has shown itself to be very interesting and attractive. Some experimental results have revealed that the superconducting mechanism could be unconventional. In this talk I will survey our recent progress of both material synthesizing and physical properties of this rich family. We have made several major contributions to the synthesizing of new pnictide superconductors. (1) Fabrication of the hole doped RE1−xSrxFexAsO samples (RE=La and Pr); (2) Fabrication of a series of new parent compounds DvFeAsF (Dv=divalent metals: Sr, Ca, Eu etc.) and many new superconductors with Tc beyond 50 K by doping electrons into the system; (3) Invention of the new material (Sr3Sc2)Fe2As2 with rather large spacing distance between the FeAs planes. We have successfully grown the NdFeAsO1−xFex and Ba1−xKxFe2As2 single crystals. It is found that the anomalous electron scattering in the normal state cannot be simply attributed to the multiband effect. The influence given by the magnetic correlation may play an important role. Specific heat, lower critical field and point contact tunneling all indicate the unconventional superconductivity and multigap features, while the paring symmetry of the superconducting gap may be a non-trivial issue. In the 1111 phase, the superfluid density is rather low and contains probably a nodal feature. While in the 122 phase, both the superfluid density and the quasiparticle density of states is about 5-10 times higher than that in the 1111 phase. An s-wave component was found in the 122 phase. I will also report the measurements on anisotropy, critical current density, critical fields and vortex phase diagram. Small anisotropy, high upper critical field and fish-tail effect (in 122) were observed. All these suggest very good potential applications. In collaboration with Gang Mu, Zhaosheng Wang, Huiqian Luo, Huan Yang, Xiuyu Zhu, Ying Jia, Yonglei Wang, Fei Han, Bing Zeng, Bing Shen, Cong Ren, Lei Shan.
3:42PM D35.00003 Determination of the phase diagram of the electron doped superconductor Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$\textsuperscript{1}, JIJUN-HAW CHU, JAMES ANALYTIS, CHRIS KUCHARCZYK, IAN FISHER, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University — Systematic measurements of the resistivity, heat capacity, susceptibility and Hall coefficient are presented for single crystal samples of the electron-doped superconductor Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$. These data delineate an $x-2\theta$ phase diagram in which the single magnetic/structural phase transition that is observed for undoped BaFe$_2$As$_2$ at 134 K appears to split into two distinct phase transitions, both of which are rapidly suppressed with increasing Co concentration. Superconductivity emerges for Co concentrations above $x > 0.025$, and appears to coexist with the broken symmetry state up to $x \sim 0.06$. The optimal $T_c$ appears to coincide with the Co concentration at which the magnetic/structural phase transitions are totally suppressed. Superconductivity is observed for a further range of Co concentrations, before being completely suppressed for $x \sim 0.18$ and above. The form of this $x-2\theta$ phase diagram is suggestive of an association between superconductivity and a quantum critical point arising from suppression of the magnetic and/or structural phase transitions.

\textsuperscript{1}This work is supported by the DOE, Office of Basic Energy Sciences, under contract no. DE-AC02-76SF00515

3:54PM D35.00004 The magnetic and superconducting phase diagram of PrFeAs$_2$O$_{1-x}$\textsubscript{F$_x$}\textsuperscript{1}, COSTEL R. ROTUNDU, STEPHEN D. WILSON, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, BYRON K. FREELON, Department of Physics, University of California, Berkeley, CA 94720, USA, EDITH BOURRET-COURCHESNE, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, ROBERT J. BIRGENEAU, Department of Physics, University of California / Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA. — The single crystal phase diagram of the newly discovered iron pnictide superconductors RFeAsO$_{1-x}$F$_x$ (R=rare-earth) is of great interest and with implications in the understanding of the nature of superconductivity (SC) itself. Predicted by ab initio calculations \cite{1} and pointed by resistivity measurements \cite{2}, the relevance of a quantum critical point remains controversial in the light of the structural phase transition between the magnetic SDW and SC \cite{3}. We present a detailed magnetic and superconducting phase diagram of PrFeAsO$_{1-x}$F$_x$, as inferred from magnetic susceptibility and resistivity measurements. References: [1] G. Giovannetti et al., Physica B 403, 3653 (2008) [2] R. H. Liu et al., Phys Rev Lett 101, 087001 (2008) [3] H. Luetkens et al., cond.mat:0806.3533

4:06PM D35.00005 Doping-Driven Collapse of the SDW Correlation Gap in SmFeAsO$_{1-x}$F$_x$\textsuperscript{1}, J.B. KEMPER, SCOTT C. RIGGS, Z. STEGEN, G.S. BOEBINGER, National High Magnetic Field Laboratory - Florida State University, R.D. MACDONALD, F.F. BALAKIREV, Y. KOHAMA, A. MIGLIORI, National High Magnetic Field Laboratory - Los Alamos National Laboratory, H. CHEN, R.H. LIU, X.H. CHEN, Hefei National Laboratory and University of Science and Technology of China — We have investigated the Hall resistivity, $\rho_{xy}$, of polycrystalline SmFeAsO$_{1-x}$F$_x$ for four different fluorine concentrations from the onset of superconductivity through the collapse of the structural phase transition. For the two more highly-doped samples, $\rho_{xy}$ is linear in magnetic field up to 50 T with only weak temperature dependence, reminiscent of a simple Fermi liquid. For the lightly-doped samples with $x < 0.15$, we find a low temperature regime characterized $\rho_{xy}(H)$ being both non-linear in magnetic field and strongly temperature dependent even though the Hall angle is small. The onset temperature for this non-linear regime is in the vicinity of the structural phase (SPT)/spin density wave (SDW) transitions. The temperature dependence of the Hall resistivity is consistent with a thermal activation of carriers across an energy gap. The evolution of the energy gap with doping is reported.

\textsuperscript{1}Partially funded by NSF Cooperative Agreement DMR-0654118 and the state of Florida.

4:18PM D35.00006 STM Investigation of the (001) surfaces of the Parent and Co-doped BaFe$_2$As$_2$\textsuperscript{1}, S. H. PAN, A. LI, D. R. JAYASUNDARA, Y. XUAN, J. P. O’NEAL, University of Houston, Houston, Texas 77204-5002, R. JIN, E. W. PLUMMER, Louisiana State University, Baton Rouge, LA 70803-4001, R. JIN, A. S. SEFAT, M. A. MCGUIRE, B. C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — We have used a UHV Low Temperature STM to study the surface structure of the parent and the Co-doped BaFe$_2$As$_2$ single crystals. Various STM images with different structural symmetry were observed. The dominant apparent surface structure is ($\sqrt{2}$x$\sqrt{2}$)R45° for the parent compound and 1 x 2 stripe-like for the Co-doped ones. We will compare the different surface structures and discuss the identification of the atomic plane exposure and the possible origins for such variety in surface structure.

\textsuperscript{1}Funding support from Texas Center for Superconductivity at UH, Robert A. Welch Foundation, and from DOE-BES-DMSE

4:30PM D35.00007 Electronic Structure on (001) Surface of BaFe$_2$As$_2$ Parent Compound Studied with Scanning Tunneling Spectroscopy\textsuperscript{1}, D. R. JAYASUNDARA, A. LI, Y. XUAN, J. P. O’NEAL, S. H. PAN, University of Houston, Houston, Texas 77204-5002, R. JIN, E. W. PLUMMER, Louisiana State University, Baton Rouge, LA 70803-4001, R. JIN, A. S. SEFAT, M. A. MCGUIRE, B. C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Doping can drive some metallic pnictide compounds to a magnetic/structural phase transition that is observed for undoped BaFe$_2$As$_2$ at 134 K appears to split into two distinct phase transitions, both of which are rapidly suppressed with increasing Co concentration. Superconductivity emerges for Co concentrations above $x > 0.025$, and appears to coexist with the broken symmetry state up to $x \sim 0.06$. The optimal $T_c$ appears to coincide with the Co concentration at which the magnetic/structural phase transitions are totally suppressed. Superconductivity is observed for a further range of Co concentrations, before being completely suppressed for $x \sim 0.18$ and above. The form of this $x-2\theta$ phase diagram is suggestive of an association between superconductivity and a quantum critical point arising from suppression of the magnetic and/or structural phase transitions.

\textsuperscript{1}Funding support from Texas Center for Superconductivity at UH, Robert A. Welch Foundation, and from DOE-BES-DMSE

4:42PM D35.00008 Structural Investigation of the BaFe$_{2-x}$As$_2$(001) Surface Using LEED and STM\textsuperscript{1}, VON BRAUN NASCIMENTO, X.B. HE, R. JIN, E.W. PLUMMER, Louisiana State University, Baton Rouge, LA, T.Y. CHIEN, BIAO HU, GUORONG LI, University of Illinois, Knoxville, TN, M.H. PAN, J.F. WENDELKEN, A.S. SEFAT, M.A. MCGUIRE, B.C. SÀLES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, TN, ANG LI, DILUSHAN R. JAYASUNDARA, YI XUAN, JARED O’NEAL, SHUHENG PAN, University of Houston, Houston, TX BaFe$_2$As$_2$, a parent compound to one of the newly discovered high-$T_c$ superconductors, presents very interesting physical properties such as a structural transition occurring prior to the formation of a spin density wave. It is surely of interest to investigate the effect of breaking the symmetry by creating a surface. Single crystals of BaFe$_2$As$_2$ were cleaved in vacuum exposing a (001) surface. Quantitative LEED I-V measurements and low-temperature STM topography revealed an ordered As surface with disordered Ba atoms present. LEED shows a clear (1 x 1) periodicity with a surface structure slightly different than the bulk. STM reveals a weak C(2 x 2) periodicity. We will explore the possibility that the C(2x2) STM image is electronic in origin.

\textsuperscript{1}Supported in part by Division of Materials Sciences and Engineering, DOE, EWP, GL, & TYC have also received support from NSF and DOE (DMS&E) (NSF-DMR-0451163).
4:54PM D35.00009 Temperature and Spatial Dependence of the Superconducting and Pseudogap of NdFeAsO$_{0.8}$F$_{0.14}$, X.B. HE, Louisiana State University, Baton Rouge, LA, M.H. PAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, G.R. LI, University Of Tennessee, Knoxville, TN 37996, J.F. WENDELKEN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, R.Y. JIN, Louisiana State University, Baton Rouge, LA 70803, A.S. SEFAT, M.A. MCGUIRE, B.C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, TN 37831, E.W. PLUMMER, Louisiana State University, Baton Rouge, LA 70803 — Scanning tunneling microscopy/spectroscopy are used to investigate the superconducting gap and pseudogap of Fe based high-Tc superconducting material NdFeAsO$_{0.8}$F$_{0.14}$ at various temperatures from 17 K to 150 K. The superconducting gap (SG) in the tunneling spectra follows the BCS prediction and closes at Tc of the bulk material. Surprisingly, a pseudogap (PG) opens abruptly just above Tc and closes at 120 K, strongly suggesting that the SG and PG states have competing order parameters in contrast to the cuprates. The PG state may be related to spin fluctuations in the doped materials. Research was supported in part at ORNL by Laboratory Directed Research and Development funds and by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US DOE.

5:06PM D35.00010 Scanning Tunneling Spectroscopy and Vortex Imaging in the Iron-Pnictide Superconductor BaFe$_{1.8}$Co$_{0.2}$As$_2$, YI YIN, M. ZECH, T.L. WILLIAMS, Harvard University, X.F. WANG, G. WU, X.H. CHEN, University of Science and Technology of China, J.E. HOFFMAN, Harvard University — We present an atomic resolution scanning tunneling spectroscopy study of superconducting BaFe$_{1.8}$Co$_{0.2}$As$_2$ single crystals in magnetic fields up to 9 Tesla. At zero field, a single gap with coherence peaks at 2Δ = 6.25 meV is observed in the density of states. At 9 T and 6 T, we image a disordered vortex lattice, consistent with isotropic, single flux quantum vortices. Vortex locations are uncorrelated with strong scattering surface impurities, demonstrating bulk pinning. The vortex-induced sub-gap density of states fits an exponential decay from the vortex center, from which we extract a coherence length ξ = 27.6 ± 2.9 Å, corresponding to an upper critical field Hc2 = 43 T.

3This work is supported by the NSF (DMR-0508812) and the AFOSR (FA9550-05-1-0371). T.L.W. acknowledges support from an NDSEG fellowship.

5:18PM D35.00011 STM measurements on iron pnictides, ZHANYBEK ALPICHSHEV, Stanford — Some results of scanning tunneling microscopy/spectroscopy of cobalt doped pnictides at different doping levels are presented.

Monday, March 16, 2009 2:30PM - 5:30PM –
Session D36 DCMP: Carbon Nanotubes: Low Temperature Electronic Properties

2:30PM D36.00001 Non-equilibrium tunneling spectroscopy in carbon nanotubes, NADYA MASON, YUNG-FU CHEN, TRAVIS DIRKS, University of Illinois at Urbana-Champaign, GASSEME AL-ZOUBI, NORMAN BIRGE, Michigan State University — We report measurements of the non-equilibrium electron energy distributions in carbon nanotubes. Carbon nanotubes can be considered model one-dimensional systems whose transport is strongly affected by electron interactions. Using tunneling spectroscopy via a superconducting probe, we have studied electron energy distribution functions, and hence inelastic electron scattering, in nanotubes that have bias voltages applied between their ends. We find that at low temperatures, electrons interact weakly in nanotubes of a few microns channel length, independent of end-to-end conductance values. Surprisingly, the energy relaxation rate can increase substantially when the temperature is raised to only 1.5 K. In general, tunneling spectroscopy with a superconducting probe may be a powerful new tool for characterizing electron behavior in carbon nanotubes.

1Work supported by the DOE under DE-FG02-07ER46453 through the FS-MRL and the NSF under DMR-0405238 and 0705213.

2:42PM D36.00002 Method for determining the conductance tensor of quantum junctions from the ground state alone, ARMIN RAHMANI, CHANG-YU HOU, CLAUDIO CHAMON, Boston University, IAN AFFLECK, University of British Columbia — Conductance is related to dynamical correlation functions and is considered a non-equilibrium quantity. Here we propose a method to obtain the small-bias low-temperature conductance tensors of quantum junctions through equilibrium calculations such as time-independent DMRG. Using the dependence of a finite system ground state energy on the boundary conditions, we determine the junction conductance by finding the S-matrix. The method is applicable to interacting junctions connected to an arbitrary number of non-interacting leads.

2DOE Grant DE-FG02-06ER46316

2:54PM D36.00003 Transition from the Sequential to the Resonant Tunneling in a Dissipative Environment, YURIY BOMZE, HENOK MEBRAHTU, IVAN BORZENETS, ALEX MAKAROVSKI, GLEB FINKELSTEIN, Duke University — We study the shape of the single-electron conductance peaks in a quantum dot coupled to a dissipative environment. In the regime of sequential tunneling through a single quantum level, the peak height increases as the temperature is lowered, although due to the dissipative environment it scales slower than the conventional 1/T. As the temperature is lowered further into the resonant tunneling regime, the peak width approaches saturation, while the peak height starts to decrease. To our knowledge, the non-monotonic peak height dependence on temperature is experimentally observed for the first time. We associate this behavior with coherent tunneling through a single quantum level in the presence of dissipative environment.

3:06PM D36.00004 Possible electric-field induced one dimensional excitonic insulators in carbon nanotubes pairs, JAY SAU, University of California Berkeley and MSD Lawrence Berkeley National Laboratory, MARVIN COHEN, University of California, Berkeley and MSD, Lawrence Berkeley National Laboratory — Recently there has been significant interest in the possibility of realizing excitonic insulator states in semiconducting systems in electric fields. Using a tight-binding formulation of the GW and Bethe-Salpeter methods parametrized from first-principles density functional theory calculations, we show that an electric field strength of 0.06 eV/A fails to close the quasiparticle gap of the system but closes the excitonic gap. This can cause a phase transition of the system into an excitonic phase where the ground state is populated with a quasi-one dimensional repulsive gas of excitons. Such a state provides a realization of a one-dimensional excitonic insulator phase with a spin degree of freedom which can lead to novel phases. We discuss some of the properties of the resulting excitonic phase and the transition and also discuss how similar properties may be observed in experiments on nanotube bundles.

3This work was supported by NSF Grant No. DMR07-05941 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been
3:18PM D36.00005 A recursion formula for the local density of states in finite Luttinger liquids1, SEBASTIAN EGGERT, IMKE SCHNEIDER, Univ. of Kaiserslautern, Germany — The local density of states (LDOS) in quantum wires is one of the most central quantities for the experimental verification of the predictions from Luttinger Liquid theory. By now, it has been well understood how boundaries lead to a crossover of powerlaws in the LDOS as a function of position and energy. It is also possible to calculate the LDOS for individual levels in finite wires analytically and numerically. However, the connection from finite wavefunctions to a semi-infinite powerlaw description remains unclear. We now present a simple recursion formula that ties together both limits and even allows to express the crossover of powerlaws in a closed analytic form in terms of hypergeometric functions. With the help of the formula it is now also possible to calculate the LDOS of long range interacting systems explicitly.

1With special thanks to OPTIMAS and the DFG funded "Transregio 49" and the "graduate school of excellence MATCOR"

3:30PM D36.00006 Superconducting Tunneling Spectroscopy of a Carbon Nanotube Quantum Dot1, TRAVIS DIRKS, YUNG-FU CHEN, NADYA MASON, Department of Physics and Materials Research Laboratory, University of Illinois, NORMAN DIRGE, Department of Physics and Astronomy, Michigan State University. We report results on tunneling spectroscopy of a carbon nanotube quantum dot. Using a three-probe technique that includes a superconducting tunnel probe, we map out changes in conductance due to band structure, excited states, and applied bias. We also see features due to the unique nature of the superconducting probe, including enhancement of weak tunneling processes. In addition, we see conduction inside the superconducting gap when an end to end bias is applied, which suggests some inelastic, possibly assisted, tunneling process inside the quantum dot.

3:42PM D36.00007 ABSTRACT WITHDRAWN —

3:54PM D36.00008 A DMRG approach to impurities and interactions in carbon nanotubes, ALEXANDER STRUCK, University of Kaiserslautern, SEBASTIAN REYES, University of Kaiserslautern and Pontificia Universidad Catolica de Chile, SEBASTIAN EGGERT, University of Kaiserslautern — Carbon nanotubes (CNTs) are well suited to study strong electronic correlations in quasi-one-dimensional systems experimentally and theoretically. Of particular interest is the interplay of interactions between the conducting electrons and impurities in the nanotube. Impurities include the boundaries of short tubes as well as structural imperfections such as the Stone-Wales lattice distortion. Interactions can lead to different phases of the electron liquid, depending on their range and strength, and can produce quasi-localized ground states of e.g. the Mott insulator type or a charge density wave. Here we discuss a systematic approach using the density-matrix renormalization group (DMRG) method to treat a recently derived lattice model for a single-wall armchair CNT with short-range interactions and a Stone-Wales impurity. We show interaction driven modifications to the expected density patterns that can lead to anomalous Friedel oscillations around the impurity.

4:06PM D36.00009 Zero-bias anomalies in multi-section carbon nanotube FETs1, YANFEI YANG, GEORGY FEDOROV, Department of Physics, Georgetown University, SERHII SHAFRANIUK, Department of Physics and Astronomy, Northwestern University, RUPERT LEWIS, BENJAMIN COOPER, CHRISTOPHER LOBB, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, PAOLA BARBARA, Department of Physics, Georgetown University — Carbon nanotube field effect transistors (CNFETs) with high transparency contacts show maxima of differential conductance at zero bias voltage [1]. These zero-bias anomalies (ZBAs) occur at large negative gate voltages and in narrow gate voltage ranges (about 1 V wide). Our proposed explanation is superconductivity in the nanotubes, occurring when the gate voltage shifts the Fermi energy into van Hove singularities of the electronic density of states. Here we probe this scenario using 3 FETs fabricated from different sections of one semiconducting carbon nanotube. Source and drain electrodes were patterned by e-beam lithography to achieve FET lengths of 500 nm, 1500 nm and 7000 nm, respectively. All devices showed high transparency contacts to their Pd electrodes. We report the observation of pronounced ZBAs in the multi-section CNFETs, their magnetic field (up to 7 T) and temperature evolution, and the modulation on the ZBAs by Fabry-Perot oscillation. [1] J. Zhang et al., Zero-bias anomaly and possible superconductivity in single-walled carbon nanotubes, Phys. Rev. B, 74, 155414 (2006).

1This work was supported by NSF (grant nos: DMR0239721 and DMR 0521170).

4:18PM D36.00010 Interacting resonant level side-coupled to a Luttinger liquid: Duality to resonant tunneling, MOSHE GOLDSTEIN, RICHARD BERKOVITS, The Minerva Center, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel. — We study a model of a single level quantum dot side-coupled to a Luttinger liquid wire by both hopping and interactions. By canonical transformations and a Coulomb gas mapping, we prove a duality between this problem and that of resonant tunneling through a level connecting the edges of two wires with the inverse Luttinger liquid parameter $g$. The two systems thus have complementary transport properties: when one is conducting the other is insulating, and vice-versa. Using this result, as well as an exact solution at $g = 2$ and Monte-Carlo simulations on the Coulomb gas, we fully characterize the system's conductance. It exhibits an anti-resonance as a function of the level energy, whose width vanishes (enhancing transport) as a power law at low temperatures and bias voltages for $g > 1$, while diverging (suppressing transport) for $g < 1$. Level population is shown to be either a linear, a power law, or a discontinuous function of a small level energy, depending on the parameters.

4:30PM D36.00011 Wigner crystal vs. Friedel oscillations in the 1D Hubbard model1, STEFAN SOEFFING, Univ. of Kaiserslautern, Germany, MICHAEL BORTZ, Univ of Kaiserslautern, Germany, SEBASTIAN EGGERT, Univ. of Kaiserslautern, Germany — We investigate the ground state density distribution of the Hubbard model in a finite one-dimensional wire. For weak interactions we find the expected Friedel oscillations, but for low filling a distinct Wigner crystal state can be observed. Although there cannot be a phase transition in a 1D system we observe a well-defined crossover into a Wigner crystal region with different physical behavior even for relatively weak short range interactions. The combination of Luttinger liquid theory and numerical Density Matrix Renormalization Group (DMRG) calculations allows a quantitative analysis of the crossover as a function of system length, lattice filling, and interaction strength.

1With special thanks to OPTIMAS and the DFG funded "Transregio 49" and the "graduate school of excellence MATCOR"
4:42PM D36.00012 Mott Insulating State in Ultra-clean Carbon Nanotubes, VIKRAM DESHPANDE, Caltech, BHUPESH CHANDRA, ROBERT CALDWELL, Columbia University, DMITRY NOVIKOV, Yale University, JAMES HONE, Columbia University, MARC BOCKRATH, Caltech — The Mott insulating state is a manifestation of strong electron interactions in nominally metallic systems. Using transport spectroscopy, we show that an energy gap exists in nominally metallic carbon nanotubes, and occurs in addition to the band-gap in small-band-gap nanotubes, indicating that carbon nanotubes are never metallic. This gap has a magnitude ~10-100 meV and nanotube radius dependence ~1/r, in good agreement with predictions for a nanotube Mott insulating state. We also observe neutral excitations within the gap, as predicted for this state. Our results underscore nanotubes’ exceptional capabilities for studying correlated electron phenomena in 1D.
Ref. V. V. Deshpande et al., Science (in press)

1Current affiliation: Columbia University

4:54PM D36.00013 Superconductivity in thin films of boron-doped carbon nanotubes, J. HARUYAMA, N. MURATA, Aoyama Gakuin Univ., J. REPPERT, A. RAO, Clemson Univ., T. KORETSUNE, S. SAITO, Tokyo Institute of Technology — It is well known that the small mass of carbon can promote high transition temperature (T_c) in BCS-type superconductivity (SC). Recently, new carbon-based superconductors with order of T_c of ~10K [1, 2] were discovered and higher T_c has been expected. In particular, the SC in a carbon nanotube (CNT) is attracting considerable attention [3]. We reported that entirely end-bonded multi-walled CNTs could show SC with T_c = 12K, previously [4]. In contrast, it had problem in reproducibility, because correlation with carrier doping was not clarified. Moreover, none has succeeded substitutional carrier doping into CNTs and also revealed the correlation with SC. Here, we report on the Meissner effect found in thin films consisting of assembled boron-doped single-walled CNTs [5]. We reveal that only highly homogeneous CNT films consisting of low boron concentration leads to evident Meissner effect with T_c = 12 K. The first-principles electronic-structure study of the B-SWNT strongly supports these results. [1] T. E. Weller et al., Nature Physics 1, 39 (2005), [2] E. A. Ekimov et al., Nature 428, 542 (2004), [3] M. Kociak et al., Phys. Rev. Lett. 86, 2416 (2001), [4] I. Takesue, J.Haruyama, et al., Phys. Rev. Lett. 96, 057001(2006), [5] N.Murata, J.Haruyama, et al., Phys.Rev.Lett. 101, 027002 (2008)

5:06PM D36.00014 Fabrication and transport properties of size tunable single-walled carbon nanotube quantum dots, PAUL STOKES, YODCHAY JOMPOL, SAIFUL I. KHONDAKER, University of Central Florida, Nanoscience Technology Center and Dept of Physics — Single electron transistors (SETs) have attracted considerable attention because of their potential as a building block for quantum based nanoelectronic devices. However fabrication of reproducible and controllable quantum dot sizes that can operate at high temperature is challenging. We developed a novel technique for the fabrication of size tunable and controllable quantum dot using single-walled carbon nanotube (SWNT) [1]. Our technique is based on the formation of two tunnel barriers of controllable separation by naturally bending SWNT at the edges of a raised local gate. A SWNT is placed on a local Al/Al2O3 bottom gate of width L, and then contacted with Pd source and drain electrodes of 1 μm separation on Si/SiO2 substrates. The Al gate serves three purposes: (i) it acts as a “mechanical template” to define two tunnel barriers at the edges by naturally bending the nanotube due to van der Walls interactions with the substrate, (ii) the width of the gate defines the size (L) of the quantum dot, and (iii) it acts as a local bottom gate to control the operation of the SET device. Using this approach we fabricated SETs of different sizes down to 50 nm. We present detailed fabrication procedures and low temperature transport studies of these SET devices. [1] P. Stokes and S. I. Khondaker, APL 92, 262107 (2008)

5:18PM D36.00015 Conductance of a Conjugated Molecule with Carbon Nanotube Contacts, NOLAS BRUQUE, University of California, Riverside, KHALID ASHRAF, THOMAS HELANDER, ROGER LAKE — Quantitative predictions of the energy levels is a well-known weakness of density functional theory (DFT). To understand the HOMO level alignment of a π-cruciform molecule [1] with the Fermi level of a carbon nanotube (CNT) contact, we have performed quantum chemical calculations of the adiabatic ionization potential (IP) of the central molecule. The adiabatic IP of the molecule is -5.86 eV. The image charge potential, calculated using our fully self-consistent DFT - Recursive Green Function (RGF) approach, is 0.7 eV. Treating the image potential as a self-energy correction to the IP, the HOMO energy level is at -5.16 eV which is comparable to the intrinsic CNT Fermi level at -5 eV. The above considerations of the energy level alignments, combined with the DFT-RGF analysis of the molecular orbitals and transmission spectrum, indicate that the HOMO resonance lies within the 50 meV energy window created by the experimental source-drain bias. This appears to be the most likely scenario that would give rise to the relatively small resistance of 6 MΩ. 1. X. Guo, et. al. Science, 311, 356 (2006).

Monday, March 16, 2009 2:30PM - 5:30PM —
Session D37 DCP: Focus Session: Fundamental Developments in Density Functional Theory

2:30PM D37.00001 Bounds on the correlation energy of Coulomb interacting systems: How negative does E_c get, and what does this imply for approximate density functionals, KLAUS CAPELLE, University of Sao Paulo, Brazil — The indirect part of the Coulomb interaction energy of a three-dimensional many-fermion system has a lower bound in terms of a power of the particle density, known as the Lieb-Oxford bound. This bound can be reformulated as a bound on the correlation energy, and in this reformulated version is an ingredient in the construction of many modern density functionals. In this talk, I describe several recent investigations and refinements of this bound: (i) an empirical analysis strongly suggesting that the bound can be tightened without losing its universality [collaboration: Mariana Odashima], (ii) the construction of a particle-number dependent version of the bound and an exploration of its consequences for PBE GGA [collaboration: Mariana Odashima and Sam Trickey], (iii) a simplified scaling derivation of the power law in the bound, and its application to construct similar bounds also for one- and two-dimensional systems [collaborators: César Proetto, Esa Räsänen and Stefano Pittalis], and (iv) a connection between the Lieb-Oxford bound and common hybrid functionals, providing an alternative rationale for why these functionals work, as well as a possible route for the construction of improved beyond-GGA functionals [collaborator: Mariana Odashima].

1Supported in part by grants from FAPESP and CNPq.
3:06PM D37.00002 Van der Waals Interactions in Density-Functional Theory. AXEL BECKE, Dalhousie University — The application of conventional GGA, and meta-GGA, density functionals to van der Waals complexes is fraught with difficulties. Conventional functionals do not contain the physics of the dispersion interaction. To make matters worse, the exchange part alone can yield anything from severe over-binding to severe over-repulsion depending on the choice of functional. We rectify these problems by - adding a dispersion term with nonempirical C6, C8, and C10 dispersion coefficients (the Becke-Johnson dispersion model), and - selecting a GGA exchange functional (PW86, also nonempirical) that gives excellent agreement with exact Hartree-Fock repulsion curves. The result is a simple GGA+dispersion theory giving excellent noble-gas pair interaction energies for He through Kr with only two adjustable parameters in the dispersion cutoff.

3:42PM D37.00003 Van der Waals interactions in density functional theory1, DAVID C. LANGRETH, Rutgers University — The van der Waals density functional which we introduced half a decade ago1, and its self-consistent generalization2 will be briefly reviewed. There are many collaborators in the application review that will follow, not only those who worked in the physics department at Rutgers1, but also at Denmark Technical University3, the chemistry department at Rutgers3, and most recently at the University of Texas at Dallas4. I will expand on our recent review article5 which hopefully will be published before the present talk, and include applications by other groups not listed below. If possible, I will also review results from a more recent collaboration to study nucleosomal DNA and beyond.

4:18PM D37.00004 Accurate van-der-Waals interactions from (semi)-local density functional theory , ALEXANDRE TKATCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — Non-covalent forces, such as hydrogen bonding and van der Waals (vdW) interactions, are crucial for the formation, stability and function of molecules and materials. At present, vdW interactions can only be satisfactorily accounted for by high-level quantum-chemical wave function or by the Quantum Monte Carlo (QMC) method. In contrast, (semi)-local DFT and Hartree-Fock approximation fail for the description of vdW forces. We present a parameter-free method for describing the long-range vdW interaction in (semi)-local DFT. The leading C6 coefficients are derived from the electron density of a molecule/solid and accurate reference values for the free atoms. The mean absolute error in the C6 coefficients is 5.5% when compared to accurate experimental values for 1225 intermolecular pairs. We show that the C6 coefficients depend strongly on the bonding type and geometry of molecules/solids. Finally, we analyze the vdW radii and the damping function in the C6R−6 correction method for DFT calculations.

4:30PM D37.00005 Efficient van der Waals density functional interactions1, JOSE M. SOLER, GUILLERMO ROMAN-PEREZ, Univ. Autonoma de Madrid — The LDA and GGA functionals are the non empirical methods of choice for large system calculations, but they cannot describe nonlocal dispersion forces. This limits severely their application to many systems of large interest like molecular solids and liquids, physisorbed molecules, and interactions between biological molecules. Several schemes have been proposed to add ad-hoc atom-atom or atom-electron potentials. But dispersion is an electron-electron correlation effect, that must be described by an appropriate density functional, such as that proposed by Dion et al (PRL 92, 246401 (2004)). It is a true universal and general-purpose DFT functional that describes semiquantitatively the week dispersion interactions, without compromising the accuracy of the best GGA functionals for stronger bonds. Its direct evaluation for large molecular systems is very expensive, however, because it requires a double integral in real space. We present a new implementation that avoids this N2 scaling by applying a density-2D convolution technique to an accurately interpolated kernel. The resulting method scales as N log N and it allows to perform vdW-DFT simulations of essentially any system that can be simulated with GGA.

4:42PM D37.00006 The discontinuous nature of the exchange-correlation functional — critical for strongly correlated systems, PAULA MORI-SANCHEZ, ARON COHEN, WEITAO YANG, Duke University — Standard approximations for the exchange-correlation functional have been found to give big errors for the linearity condition of fractional charges, leading to delocalization error, and the constancy condition of fractional spin, leading to static correlation error. These two conditions are now unified for states with both fractional charge and fractional spin: the exact energy functional is a plane, linear along the fractional charge coordinate and constant along the fractional spin coordinate with a line of discontinuity at the integer. This sheds light on the nature of the derivative discontinuity and calls for explicitly discontinuous functionals of the density or orbitals that go beyond currently used smooth approximations. This is key to understand the physics of strongly correlated systems within DFT, for example the band-gap of Mott insulators. [arXiv:0809.5108]

4:54PM D37.00007 Advances in Local Hybrid Functionals, ALEKSEY ARBUZNIKOV, MARTIN KAUPP, HILKE BAHMANN. University of Wuerzburg — Local hybrids provide a promising new generation of exchange-correlation functionals for the simultaneous accurate description of various properties (atomization energies, reaction barrier heights, INMR chemical shifts, energetics of transition-metal systems, etc.) Compared to traditional (global) hybrids (e.g., B3LYP), instead of a constant exact-exchange admixture, local hybrids employ a position-dependent one. The latter is governed by a so-called local mixing function (LMF), and this is the crucial quantity controlling the performance of local hybrids. Here we present and compare new results obtained with LMFs derived both in a semiempirical way and using ab initio considerations, e.g., the adiabatic local correlation formalism. The former approach yields better results, while the latter brings valuable insights into the performance and limits of local hybrids.

1 This work has been founded by grant FIS2006-12117 from the Spanish Ministry of Science.


5:06PM D37.00008 Calculation of functional derivatives with respect to the external potential, NICK SABLON, TIM FIEVEZ, FRANK DE PROFT, PAUL W. AYERS, PAUL GEERLINGS, Vrije Universiteit Brussel — Apart from its many computational advantages, density functional theory (DFT) presents a conceptual framework for the reactivity and stability interpretation of chemical systems. The central idea is to identify chemical concepts with first and higher order (functional) derivatives of the electronic energy with respect to the number of electrons N and the external potential \( v(r) \). The local interpretation of chemical reactivity is generally given in an exact theory. Practical DFT calculations make however use of approximate exchange-correlation functionals for which the DFT concepts can only correctly be obtained by an effective evaluation of the electronic derivatives. A recent methodology for the calculation of functional derivatives with respect to \( v(r) \) is presented. Results are shown for a wide range of molecules among which substituted benzenes. A reactivity description of the alkaline earth oxides’ (100) surface is expounded on as well.


5:18PM D37.00009 Simple Illustration of Partition Theory, ADAM WASSERMAN, Department of Chemistry - Purdue University, MORREL COHEN, Department of Physics - Rutgers University, and Department of Chemistry - Princeton University, KIERON BURKE, Department of Chemistry - UC-Irvine, ROBERTO CAR, Department of Chemistry - Princeton University — In Partition Theory (PT) \cite{Wasser2007} the density of a system is decomposed exactly into a superposition of the densities of its parts through the introduction of a common partition potential acting on each of the parts as if they were isolated. In this talk we illustrate PT on a simple one-dimensional model of a heteronuclear diatomic molecule. We show that a sharp definition for the charge of the fragments emerges from PT, and that the ensuing population analysis can be used to study how charge redistributes during dissociation. By studying the preservation of the shapes of the parts as different parameters of the model are varied, we address the issue of transferability of the parts. We find good transferability within the chemically meaningful parameter regime, raising hopes that PT will prove useful in chemical applications.


2:30PM D38.00001 Exciton migration and fluorescence quenching in photosystem II, LEONAS VALKUNAS, Institute of Physics, Savanoriu 231, 02300 Vilnius and Theoretical Physics Chair, Vilnius University, Sauletekio 9, build. 3, 10222 Vilnius, Lithuania — When exposed to excess light illumination photosynthetic organisms switch into a photoprotective quenched state where the excess energy is safely dissipated as heat. It was recently discovered that the main light-harvesting complex of plants, LHCII, plays a key role in the dissipation of excess energy. Here we demonstrate that the excitation kinetics in the quenched state can be described by a simple model, which assumes specific trapping centers to be present in the system \cite{Holt2007}. In order to explain the experimental results exciton-exciton annihilation is taken into account. To verify the effectiveness of the non-photochemical quenching center, possessing a short lifetime, in preventing the excess excitations from reaching the reaction center, the studies of the excitation quenching depending on positioning and origin of the quencher in the antenna complexes are also considered.


3:06PM D38.00002 Environment-assisted quantum transport in photosynthetic complexes, ALAN ASPURU-GUZIK, Harvard University — Transport phenomena at the nanoscale are of interest due to the presence of both quantum and classical behavior. In this work, we demonstrate that quantum transport efficiency can be enhanced by a dynamical interplay of the system Hamiltonian with the pure dephasing dynamics induced by a fluctuating environment. This is in contrast to fully coherent hopping that leads to localization in disordered systems, and to highly incoherent transfer that is eventually suppressed by the quantum Zeno effect. We study these phenomena in the Fenna-Matthews-Olson protein complex as a prototype for larger photosynthetic energy transfer systems. We also show that disordered binary tree structures exhibit enhanced transport in the presence of dephasing. We address the question of the role of quantum coherence in the energy transfer in the FMO complex and discuss details about the theoretical modeling of photosynthetic complexes and organic photovoltaic materials.

3:42PM D38.00003 Engineering Efficient Exciton Energy Transfer in Artificial Arrays, LESLIE VOGT, ALEJANDRO PERDOMO, SEMION SAIKIN, ALAN ASPURU-GUZIK, Harvard University — A critical component of light harvesting devices is efficient transfer of excitonic energy. Biological systems have optimized this process over time for the particular molecular components involved. Understanding this energy transfer in model arrays will allow us to engineer new materials for solar cell technology. In particular, we explore a perturbative approach to optimize both coherent and incoherent transport in small arrays. By following the evolving coherences and populations over time using a density matrix formalism, we gain an intuition about the importance of coherent processes in exciton transfer in natural and designed light harvesting systems.

3:54PM D38.00004 Coherent Excitonic Transfer in the Fenna Matthews Olson Complex, GREGORY ENGEL, The University of Chicago — Evidence for a purely quantum mechanical mechanism of energy transfer in photosynthetic complexes was discovered in the Fenna-Matthews-Olson complex of Chlorobium tepidum in 2007. The quantum beating phenomenon observed in this complex is now much better understood. Specifically, detailed, testable microscopic models for the mechanism of this energy transfer have emerged, and precise quantum dynamical models now predict that this mechanism accounts for approximately one quarter of the energy transferred at room temperature. Further, new data indicate that this mechanism is not specific to FMO, but manifests in reaction centers of purple bacteria and antenna complexes of higher plants. A new experimental effort to observe quantum coherence at room temperature will be discussed. Specifically, by comparing population transfer rates and coherence transfer quantum beating signals, we calculate the fraction of the energy moving through the wave-like mechanism. Further, by studying the temperature dependence of the energy transfer, we elucidate the microscopic mechanism for wavelike energy transfer and be able to comment on the robustness of the mechanism. Are light harvesting proteins delicately “tuned” by evolution to support coherence transfer or should any proteinaceous environment support this mechanism? Details of the experimental apparatus, results and future experiments will be presented.

4:06PM D38.00005 Excitation transport in open quantum systems: the role of environmental correlations, MOHAN SAROVAR, YUAN-CHUNG CHENG, BIRGITTA WHALEY, University of California, Berkeley — The recent discovery of quantum coherent phenomena in photosynthetic complexes \cite{Engel2007a} has prompted several studies into the efficiency of transport processes in open quantum systems. Several of these studies have revealed a subtle interplay between coherent and decohered dynamics in the overall efficiency of transport in these open systems. Some have shown that decoherence can improve efficiency. However all studies have used simple uncorrelated models of decoherence that are not accurate for photosynthetic complex environments, which are known to be spatially and temporally correlated. In this work we investigate the role of environmental correlations in quantum transport in open systems and show that the exact nature of the correlations can have a large impact on the efficiency of energy harvesting. We illustrate our results using the Fenna-Matthews-Olson photosynthetic complex.
fluctuations in oscillatory activities significantly. Then study the extended repressilator system to investigate the effect of extra component and identify the combinatoric regulation pattern that reduces the fluctuations.

We will show how the details of the stochastic process can be characterized by a few effective parameters, which facilitates modeling but complicates interpretation of current experiments. I will show how the resulting noise can provide advantageous or deleterious phenotypic fluctuation and how noise control in the copy number control system of plasmin can change the selective pressures. This system illustrates the direct connection between molecular dynamics and evolutionary dynamics.

APAM, C2B2 — Modeling the dynamics of biological networks while respecting the intrinsic stochasticity requires accounting for intrinsic fluctuations arising from the low copy count of the constituent particles. Traditional simulation-based approaches to computing the probability distribution, rather than by directly solving for the distribution using a fast and accurate method that exploits the natural basis of the uncoupled problem from the same class. We illustrate our method on a ubiquitous biological example: linear signaling cascades. The huge efficiency gains permit optimization of information transmission over input and regulatory parameters, revealing design properties of the most informative cascades. We find, for threshold regulation, that a cascade of strong regulations converts a unimodal input to a bimodal output, that multimodal inputs are no more informative than bimodal inputs, and that a chain of DC up-regulations outperforms a chain of AC down-regulations.

Session D39 DBP GSNP: Focus Session: Noise and Fluctuations in Biochemical Networks

Monday, March 16, 2009 2:30PM - 5:18PM

2:30PM D39.00001 Stochasticity in cell biology: Modeling across levels. JUAN MANUEL PEDRAZA, Harvard University. Effective modeling of biological processes requires focusing on a particular level of description, and this requires summarizing de details of lower levels into effective variables and properly accounting for the constraints that other levels impose. In the context of stochasticity in gene expression, I will show how the details of the stochastic process can be characterized by a few effective parameters, which facilitates modeling but complicates interpretation of current experiments. I will show how the resulting noise can provide advantageous or deleterious phenotypic fluctuation and how noise control in the copy number control system of plasmin can change the selective pressures. This system illustrates the direct connection between molecular dynamics and evolutionary dynamics.

2:33PM D39.00002 Mean-field vs. Stochastic Models for Transcriptional Regulation. RALF BLOSSEY, CLAUDIU GIURANIUC, CNRS, BIOLOGICAL NANOSYSTEMS TEAM. We introduce a minimal model description for the dynamics of transcriptional regulatory networks. It is studied within a mean-field approximation, i.e., by deterministic ode's representing the reaction kinetics, and by stochastic simulations employing the Gillespie algorithm. We elucidate the different results both approaches can deliver, depending on the network under study, and in particular depending on the level of detail retained in the respective description. Two examples are addressed in detail: the repressor, a transcriptional clock based on a three-gene network realized experimentally in E. coli, and a bistable two-gene circuit under external driving, a transcriptional network motif recently proposed to play a role in cellular development.

2:36PM D39.00003 The stochastic spectral analysis of transcriptional regulatory cascades. ANDREW MUGLER, Columbia University, Physics, ALEKSANDRA M. WALCZAK, Princeton University, PCTS, CHRIS H. WIGGINS, Columbia University, APAM, C2B2. Modeling the dynamics of biological networks while respecting the intrinsic stochasticity requires accounting for intrinsic fluctuations arising from the low copy count of the constituent particles. Traditional simulation-based approaches to computing the probability distribution, rather than by directly solving for the distribution using a fast and accurate method that exploits the natural basis of the uncoupled problem from the same class. We illustrate our method on a ubiquitous biological example: linear signaling cascades. The huge efficiency gains permit optimization of information transmission over input and regulatory parameters, revealing design properties of the most informative cascades. We find, for threshold regulation, that a cascade of strong regulations converts a unimodal input to a bimodal output, that multimodal inputs are no more informative than bimodal inputs, and that a chain of DC up-regulations outperforms a chain of AC down-regulations.

2:39PM D39.00004 Tuning stochastic transition rates in a bistable genetic network. VIJAY CHICKKARNE, California Institute of Technology, CARSTEN PETERSON, Lund University, Sweden. We investigate the stochastic dynamics of a simple genetic network, a toggle switch, in which the system makes transitions between the two alternative states. Our interest is in exploring whether such stochastic transitions, which occur due to the intrinsic noise such as transcriptional and degradation events, can be slowed down/speeded up, without changing the mean expression levels of the two genes, which comprise the toggle network. Such tuning is achieved by linking a signaling network to the toggle switch. The signaling network comprises of a protein, which can exist in either an active (phosphorylated) or inactive (dephosphorylated) form, and where its state is determined by one of the genetic network components: the active form of the protein in turn feeds back on the dynamics of the genetic network. We find that the rate of stochastic transitions from one state to the other, is determined essentially by the speed of phosphorylation, and hence the rate can be modulated by varying the phosphatase levels. We hypothesize that such a network architecture can be implemented as a general mechanism for controlling transition rates and discuss applications in population studies of two differentiated cell lineages, ex: the myeloid/erythroid lineage in hematopoiesis.

2:42PM D39.00005 Optimizing information flow in small genetic networks. ALEKSANDRA M. WALCZAK, Princeton University, GASPER TKACIK, University of Pennsylvania, CURTIS G. CALLAN, WILLIAM BIALEK, Princeton University. Many of the biological networks inside cells can be thought of as transmitting information from the inputs (e.g., the concentrations of transcription factors or other signaling molecules) to their outputs (e.g., the expression levels of various genes). On the molecular level, the relatively small concentrations of the relevant molecules and the intrinsic randomness of chemical reactions provide sources of noise that set physical limits on this information transmission. Given these limits, not all networks perform equally well, and maximizing information transmission provides a candidate design principle from which we might hope to derive the properties of real regulatory networks. As a starting point, I will consider the simple case of one input transcription factor that controls many genes. I will discuss the properties of these specific small networks that can transmit the maximum information. Concretely, I will show how the form of molecular noise drives predictions not just of the qualitative network topology but also the quantitative parameters for the input/output relations at the nodes of the network. In an attempt to link these general theoretical considerations to real biological systems, I will illustrate the predictions on the example of transmission of positional information in the early development of the fly embryo.

2:45PM D39.00006 Characterizing noise in genetic oscillatory systems. BYUNGJOON MIN, KWANG-IL GOH, IN-MOOK KIM, Korea University. Quantitative understanding of fluctuations in genetic circuits is crucial for understanding living systems. Despite the recent advances in the subject, however, fluctuations in non-stationary activities such as molecular oscillations have not been much investigated yet. Here we quantify the fluctuations in periods and amplitudes of oscillation and the noise propagation in the genetic oscillatory system, the repressilator, using exact stochastic simulation. At the single protein level, we found that the fluctuation in oscillation amplitudes is larger than that in oscillation periods. Noise propagation is studied in terms of the correlations in the successive periods and amplitudes, respectively, which decay exponentially down the regulatory cascades. We then study the extended repressilator system to investigate the effect of extra component and identify the combinatoric regulation pattern that reduces the fluctuations in oscillatory activities significantly.

LOCAL CORRELATION CALCULATIONS USING STANDARD AND RENORMALIZED COUPLED-CLUSTER METHODS. PIOTR PIEUCH, WEI LIU, JEFFREY GOUR, Department of Chemistry, Michigan State University. Local correlation variants of the coupled-cluster (CC) theory with singles and doubles (CCSD) and CC methods with singles, doubles, and non-iterative triples, including CCSD(T) and the completely renormalized CR-CC(2,3) approach, are developed. The main idea of the resulting CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) methods is the realization of the fact that the total correlation energy of a large system can be obtained as a sum of contributions from the occupied orthonormal localized molecular orbitals and their respective occupied and unoccupied orbital domains. The CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) algorithms are characterized by the linear scaling of the total CPU time with the system size and embracing parallelism. By comparing the results of the canonical and CIM-CC calculations for normal alkanes and water clusters, it is demonstrated that the CIM-CCSD, CIM-CCSD(T), and CIM-CR-CC(2,3) approaches recover the corresponding canonical CC correlation energies to within 0.1 % or so, while offering savings in the computer effort by orders of magnitude. By examining the dissociation of dodecane into C_{12}H_{26} and CH_{4} and several lowest-energy structures of the (H_{2}O)_{n}, clusters, it is shown that the CIM-CC methods accurately reproduce the relative energetics of the corresponding canonical CC calculations.
4:06PM D39.00007 Purely stochastic binary decisions in cell signaling models without underlying deterministic bistabilities. Maxim N. Artymov, Massachusetts Institute of Technology, Jayajit Das, Ohio State University, Mehran Karidar, Arup Chakraborty, Massachusetts Institute of Technology — Detection of different extra-cellular stimuli leading to functionally distinct outcomes is common in cell biology, and is often mediated by differential regulation of positive and negative feedback loops that are a part of the signaling network. For cellular responses stimulated by small numbers of molecules, the stochastic effects are important. Therefore, we studied the influence of stochastic fluctuations on a simple signaling model with dualing positive and negative feedback loops. The class of models we have studied is characterized by single deterministic steady states for all parameter values, but the stochastic response is bimodal; a behavior that is distinctly different from models studied in the context of gene regulation. For small numbers of signaling molecules, stochastic effects result in a bimodal distribution for this quantity, with neither mode corresponding to the deterministic solution; i.e., cells are in “on” or “off” states, not in some intermediate state. For a large number of molecules, the stochastic solution converges to the mean-field result. When fluctuations are important, we find that signal output scales with control parameters “anomalously” compared to mean-field predictions.

4:18PM D39.00008 Fitness effects of fluctuations in biochemical networks. Sorin Tanase-Nicolae, University of Michigan — The concentration of many cellular components fluctuates not only as a response to external and internal inputs but also due to random birth and death events of individual molecules. This biochemical noise affects the capacity of every individual cell to respond and adapt to the environment. While the sources and effects of biochemical fluctuations on individual cells have been intensively studied, the effects of noise on the growth rate of a population of cells are much less understood. We present a model of the cell cycle in which the growth and division of individual cells are coupled with the noisy dynamics of their internal components. The model allows us to compute the contribution of the biochemical noise to the average growth rate of a population of cells as a function of the noise strength and the correlation time of the fluctuations. We show that, due to fluctuations, the growth rate of a population of cells is always larger than the average growth rate of a individual cell and can be larger even than a corresponding deterministic model. In many cases it is assumed that the average concentration of a cellular component is close to a value that maximizes the population growth as given by the external, environmental, conditions and the internal cellular regulation. In such cases we show that contribution of fluctuations to the growth rate is negative and increases with the sensitivity of the biochemical network to the noise sources and the noise correlation time. We also discuss how the selection pressure due to fluctuations affects the structure and parameters of genetic regulatory networks.

4:54PM D39.00009 Effects of delay and noise in a negative feedback regulatory motif. Matteo Palassini, University of Barcelona, Marta Dies, Laboratori de Bioquimica i Biofisica Computacional, Institut Municipal d’Investigació Medica, Barcelona — The small copy number of the molecules involved in gene regulation can induce nontrivial stochastic phenomena such as noise-induced oscillations. An often overlooked aspect of regulation dynamics are the delays involved in transcription and translation. Delays introduce analytical and computational complications because the dynamics is non-Markovian. We study the interplay of noise and delays in a negative feedback model of the p53 core regulatory network. Recent experiments have found pronounced oscillations in the concentrations of proteins p53 and Mdm2 in individual cells subjected to DNA damage. Similar oscillations occur in the Hes-1 and NK-kB systems, and in circadian rhythms. Several mechanisms have been proposed to explain this oscillatory behaviour, such as deterministic limit cycles, with and without delay, or noise-induced excursions in excitable models. We consider a generic delayed Master Equation incorporating the activation of Mdm2 by p53 and the Mdm2-promoted degradation of p53. In the deterministic limit and for large delays, the model shows a Hopf bifurcation. Via exact stochastic simulations, we find strong noise-induced oscillations well outside the limit-cycle region. We propose that this may be a generic mechanism for oscillations in gene regulatory systems.

5:06PM D39.00010 Individuals in the crowd: studying bacterial quorum-sensing at the single-cell level. Pablo DelFino Perez, Jonathan Young, Elaine L. Johnson, Stephen J. Hagen, University of Florida, Physics Department, Gainesville FL 32611-8440 USA — Like many bacterial species, the marine bacterium Vibrio fischeri can detect its own population density through a quorum sensing (QS) mechanism. The bacterium releases a small molecular signal – the autoinducer (AI) – into its environment: high AI concentration indicates high population density and triggers a genetic switch that, in V.fischeri, leads to bioluminescence. Although the QS behavior of bulk cultures of V.fischeri has been extensively studied, little is known about either the response of individual cells to AI signal levels or the role of noise and local diffusion in QS signaling. We have used a photon-counting camera to record the luminescence of individual V.fischeri cells immobilized in a flow cell and subject to varying concentrations of AI. We observe that light output by individual cells varies not only with bulk AI concentration, but also over time, between cells, with local (micron-scale) population density, and even with the flow rate of the medium. Most of these variations would not be evident in a bulk culture. We will present an analysis of this heterogeneity at the cell level and its implications for the role of noise in QS signaling.

3Supported by NSF MCB #0347124.

Monday, March 16, 2009 2:30PM - 5:30PM — Session D40 DBP: Nucleic Acids: Packaging, Ejection and Translocation 412

2:30PM D40.00001 Anomalous scaling of nano-pore translocation times of structured biomolecules. Malcolm Mccauley, Robert Forties, Department of Physics, Ohio State University, Ulrich Gerland, Arnold Sommerfeld Center for Theoretical Physics, University of Munich (LMU), Ralf Bundschuh, Department of Physics, Ohio State University — Translocation through a nano-pore is a new experimental technique to probe physical properties of biomolecules. A bulk of theoretical and computational work exists on how the main observable, the time to translocate a single molecule, depends on the length of the molecule for unstructured molecules. Here, we study the same problem but for RNA molecules for which the breaking of the secondary structure is the main barrier for translocation. To this end, we calculate the mean translocation time of single-stranded RNA through a nanopore of zero thickness and at zero voltage for many randomly chosen RNA sequences. We find the translocation time to depend on the length of the RNA molecule with a power law. The exponent changes as a function of temperature and exceeds the naively expected exponent of two for purely diffusive transport at all temperatures.

2:42PM D40.00002 DNA Physical Mapping via the Controlled Translocation of Single Molecules through a 5-10nm Silicon Nitride Nanopore. Derek Stein, Walter Reisner, Zhijun Jiang, Nick Hagerty, Charles Wood, Jason Chan, Brown University — The ability to map the binding position of sequence-specific markers, including transcription-factors, protein-nucleic acids (PNAs) or deactivated restriction enzymes, along a single DNA molecule in a nanofluidic device would be of key importance for the life-sciences. Such markers could provide an indication of the active genes at particular stage in a cell’s transcriptional cycle, pinpoint the location of mutations or even provide a DNA barcode that could aid in genomics applications. We have developed a setup consisting of a 5-10 nm nanopore in a 20nm thick silicon nitride film coupled to an optical tweezer setup. The translocation of DNA across the nanopore can be detected via blockades in the electrical current through the pore. By anchoring one end of the translocating DNA to an optically trapped microsphere, we hope to stretch out the molecule in the nanopore and control the translocation speed, enabling us to slowly scan across the genome and detect changes in the baseline current due to the presence of bound markers.
2:54PM D40.00003 The Effects of Bio-functionalization on Solid-state Nanopore Transport — Theory and Experiments on DNA.\textsuperscript{1} YALING LIU, ABHIJIT RAMACHANDRAN, Department of Mechanical and Aerospace Engineering, SAMIR M. IQBAL, Department of Electrical Engineering, NanoFAB Center, University of Texas at Arlington — Solid-state nanopore channels have been reported recently to show selectivity for various target bio-molecules. The surfaces of nanopore channels are functionalized to achieve such selectively. The organic molecule coatings alter the behavior of molecular transport as well as change surface energies, chemical and physical properties, and make these more bio-compatible. We present theoretical considerations of DNA-modified nanopore channels which treat the functional molecules on the surface as a combination of series of potential sites. The potential function depends on the physical interactions of two ssDNA molecules. The simulated DNA trajectories and translocation speed under various test conditions are consistent with the reported experimental data.

\textsuperscript{1}This work is supported by University of Texas at Arlington Research Enhancement Program.

3:06PM D40.00004 Nanopores as a Single-Molecule Probe for Protein-DNA Complexes, A.R. HALL, S.W. KOWALCZYK, R.M.M. SMEETS, N.H. DEKKER, C. DEKKER, Kavli Institute of Nanoscience, Delft Institute of Technology — In recent years, solid state nanopores have emerged as a productive novel technique for molecular biophysics. The electrophoretic motion of single molecules through these small-scale structures can offer insights into both conformation and charge structure. Here, we apply the method to the ReCA nucleoprotein filament — a conformation where proteins polymerize along the entire length of a double-stranded DNA. This offers a unique geometry and charge structure which we probe through a combination of translocation experiments and optical tweezer measurements. We discuss conductance blockade events that are notably larger (12 nS) than those measured for bare dsDNA (1 nS), and present force spectroscopy data showing a high level of charge screening in solution (>90%).

3:18PM D40.00005 Computational model of controlled translocation of DNA molecule through a nanopore membrane with tunable electrostatic potential, ALEXEY NIKOLAEV, MARIA GRACHEVA, Clarkson University — We present results of computational modeling of controllable DNA translocation through a nanopore in a thin electrically tunable membrane composed of two layers of n-type and p-type semiconductor materials. Membrane potential biases are used to obtain distinct electrostatic potential landscapes. The membrane-DNA system is immersed in a biased electrolyte solution under bias to induce DNA translocation. A simple charges-and-springs model is used to model polynucleotide molecule. We compare electrostatic potential landscapes of the membrane with one and more potential extrema and show how electrostatic potential landscape in the nanopore alters the control over the molecule translocation. In particular, we specify different conditions under which DNA nucleotides can be translocated through the nanopore one by one in both directions as well as paused in the nanopore.

3:30PM D40.00006 Heterogeneity in Retroviral Nucleocapsid Protein Function, CHRISTY LANDES, University of Houston — Time-resolved single-molecule fluorescence spectroscopy was used to study the human T-cell lymphotropic virus type 1 (HTLV-1) nucleocapsid protein (NC) chaperone activity as compared to that of the HIV-1 NC protein. HTLV-1 NC contains two zinc fingers with each having a CCHC binding motif similar to HIV-1 NC. HIV-1 NC is required for recognition and packaging of the viral RNA and is also a nucleic acid chaperone protein that facilitates nucleic acid restructuring during reverse transcription. Because of similarities in structures between the two retroviruses, we have used single-molecule fluorescence energy transfer to investigate the chaperoning activity of HTLV-1 NC protein. The results indicate that HTLV-1 NC protein induces structural changes by opening the transactivation response (TAR)-DNA hairpin to an even greater extent than HIV-1 NC. However, unlike HIV-1 NC, HTLV-1 NC does not chaperone the strand-transfer reaction involving TAR-DNA. These results suggest that despite its effective destabilization capability, HTLV-1 NC is not as effective at overall chaperone function as is its HIV-1 counterpart.

3:42PM D40.00007 Energetics of genome ejection from phage revealed by isothermal titration calorimetry, MEERIM JEEMBAEVA, BENGT JONSSON, MARTIN CASTELNOVO, ALEX EVILEVITCH — It has been experimentally shown that ejection of double-stranded DNA from phage is driven by internal pressure reaching tens of atmospheres. This internal pressure is partially responsible for delivery of DNA into the host cell. While several theoretical models and simulations nicely describe the experimental data of internal forces either resisting active packaging or equivalently favoring spontaneous ejection, there are no direct energy measurements available that would help to verify how quantitative these theories are. We performed direct measurements of the enthalpy responsible for DNA ejection from phage \( \lambda \), using Isothermal Titration Calorimetry. The phage capsids were “opened” in vitro by titrating \( \lambda \) into a solution with LamB receptor and the enthalpy of DNA ejection process was measured. In his way, enthalpy stored in \( \lambda \) was determined as a function of packaged DNA length comparing wild-type phage \( \lambda \) (48.5 kb) with a shorter \( \lambda \)-DNA length mutant (37.7 kb). The temperature dependence of the ejection enthalpy was also investigated. The values obtained were in good agreement with existing models and provide a better understanding of ds-DNA packaging and release mechanisms in motor-packaged viruses (e.g., tailed bacteriophages, Herpes Simplex, and adenoviruses).

3:54PM D40.00008 Inhibition of DNA ejection from bacteriophage by Mg\(^{\pm2}\) counterions, SEIL LEE, School of Physics, Georgia Institute of Technology, CATHY V. TRAN, School of Chemistry and Biochemistry, Georgia Institute of Technology, TOAN T. NGUYEN, School of Physics, Georgia Institute of Technology — The problem of inhibiting viral DNA ejection from bacteriophages by multivalent counterions, especially Mg\(^{\pm2}\) counterions, is studied. Experimentally, it is known that MgSO\(_4\) salt has a strong and non-monotonic effect on the amount of DNA ejected. There exists an optimal concentration at which the least DNA is ejected from the virus. At lower or higher concentrations, more DNA is ejected from the capsid. We propose that this phenomenon is the result of DNA overcharging by Mg\(^{\pm2}\) multivalent counterions. As Mg\(^{\pm2}\) concentration increases from zero, DNA net charge changes from negative to positive. The optimal inhibition corresponds to the Mg\(^{\pm2}\) concentration where DNA is neutral. At lower/higher concentrations, DNA genome is charged. It prefers to be in solution to lower its electrostatic self-energy, which consequently leads to an increase in DNA ejection. Our theory fits experimental data well. The strength of DNA-DNA short range attraction, mediated by Mg\(^{\pm2}\), is found to be \(-0.003 k_B T \) per nucleotide base.

4:06PM D40.00009 Osmotic pressure: resisting or promoting DNA ejection from phage? Internal capsid-pressure dependence of viral infection, ALEX EVILEVITCH, MEERIM JEEMBAEVA, Department of Biochemistry, Lund University, Sweden, SARAH KOESTER, Department of Physics, Harvard University, Cambridge, MA, MARTIN CASTELNOVO, Laboratoire de Physique, Ecole Normale Superieure de Lyon, France, DAVID WEITZ, Department of Physics, Harvard University, Cambridge, MA — Recent in vitro experiments have shown that DNA ejection from phage can be partially stopped by surrounding osmotic pressure when ejected DNA is digested by DNase I on the course of infection. We argue in this work by combination of experimental techniques (UV absorbance, pulse-field electrophoresis, and cryo-EM) that intact genome (i.e. undigested) ejection in a crowded environment is, on the contrary, enhanced or eventually complete with the help of a pulling force resulting from DNA condensation induced by the osmotic stress itself. This demonstrates that in vivo, the osmotically stressed cell cytoplasm will promote phage DNA ejection rather than resisting it. While, in vitro, the ejection depends sensitively on internal pressure within the virus capsid, the effect of internal pressure on infection of bacteria is unknown. We use microfluidics to monitor individual cells and determine the distribution of lysis due to infection as the capsid pressure is varied. The lysis probability decreases markedly with decreased capsid pressure.
and heavy fermion superconductors. The energy of the BT of the spin susceptibility is strikingly similar to the phenomenology of resonance peaks in high-Tc superconductors. We assume that the HO gap is due to a particle-hole condensate that connects nested parts of the Fermi surface with nesting vector $Q^*$. The predicted behavior in URu2Si2 and argue that a gap in the fermion spectrum will produce an incommensurate spin resonance at $Q^* = (1 - 2\pi/3)$ in the case of a B phase without pentamers does not change, while the modified A and C phases show a large drop in their breaking force to approximately the value of the B capsids. This result indicates that upon DNA packaging a structural change at or near the pentamers occurs which mechanically reinforces the capsid structure. The reported binding of proteins UL17/UL25 to the pentamers of the A and C capsids seems the most likely candidate for such capsids strengthening. Finally, the data supports the view that initiation of DNA packaging triggers the maturation of HSV-1 capsids.

3 Medizinische Hochschule Hannover, Germany

4:42PM D40.00012 Effect of ions on polymer ejection dynamics from viral capsids1. ISSAM ALI, Department of Physics, College of Science, PO Box 36, Sultan Qaboos University, Al Khod 123, Oman, DAVIDE MARENDUZZO, SÚPA, School of Physics, University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ, UK, JULIA YEOMANS, Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, UK — We present simulations investigating the impact of adding ions on the dynamics of semiflexible (DNA-like) polymers ejecting from spherical viral capsids. We find that when the DNA charge is less screened, due to, for example, the addition of monovalent ions like Na+, the resulting electric interactions give rise to larger ejection forces, speeding up the ejection process. The results suggest that DNA ejection can be controlled by tuning the salt concentration in the environment, in agreement with recent experiments. We also observe that the DNA structure inside the capsid changes when electrical forces are present, tending to become more spool-like.

5:06PM D40.00014 Electrically Gated Solid State Nanopores, ZHIJUN JIANG, WALTER REISNER, DEREK STEIN, Brown University — We are exploring the use of electrically functionalized solid-state nanopores for controlling the transport of ions and single DNA molecules in solution. We have integrated annular gate electrodes inside solid-state nanopores that can electrostatically adjust both the polarity and the density of the inner surface charge. An applied gate potential can thereby influence the density of mobile counter-ions inside a pore at low salt concentrations. Our theoretical calculations show that a 0.1 V change in the gate potential can change the pore conductance by more than a factor of 5, making the nanopore behavior similar to that of a transistor. Furthermore, the electrostatic interaction between the nanopore surface and negatively charged DNA molecules can be probed in the regime of double-layer overlap. A negatively charged inner nanopore surface should repel DNA, and limit its possibility to insert into the nanopore. Positive surface charges, on the other hand, will attract DNA, and translocation should be favored. We seek to electrostatically control the translocation of DNA through the nanopore, and thereby mimic single-molecule regulatory capabilities of biological nanopores.

5:18PM D40.00015 Structural transitions in packing of a semi-flexible chain confined in a sphere, ARTEM LEVANDOVSKY, LEONID PRYADKO, ROYA ZANDI, University of California, Riverside — We study phases and phase transitions (crossovers) between phases of a semi-flexible polymer chain confined in a spherical cavity. Such a problem is relevant to DNA or RNA packaging in viruses whose organization is characterized by both simplicity and economy. The confinement involves both energetic and entropic effects controlled by the stiffness of the chain, its length and diameter, and the sphere radius. Formation of different packing configurations and structural changes in these configurations is studied with a non-local “cluster” Monte Carlo method. We introduce several order parameters characterizing different packing symmetries and compute the corresponding probability distributions. This allows us to reconstruct the Landau free energies for these order parameters, and thus develop a simple theory of packing transitions.

Monday, March 16, 2009 2:30PM - 5:06PM — Session D41 DMP DCMP: Hidden Order and Quantum Criticality in Heavy Fermions 413

2:30PM D41.00001 Incommensurate spin resonance in URu2Si2. JIAN XIN ZHU, ALEXANDER BALATSKY, ATHANASIOS CHANTIS, HARI DAHAL, LANL, DAVID PARKER, NRL — The nature of the hidden order (HO) in URu2Si2 below $T_{HO} = 17.5$K has been a puzzle for a long time. Here we propose to search for the spin resonance as a tool to elucidate the nature of the HO. We considerinelastic neutron scattering in URu2Si2 and argue that a gap in the fermion spectrum will produce an incommensurate spin resonance at $Q^{*} = (1 pm 0.4, 0.0)$ at $\omega_{res} = 4.6$ meV. We assume that the HO gap is due to a particle-hole condensate that connects nested parts of the Fermi surface with nesting vector $Q^{*}$. The predicted behavior of the spin susceptibility is strikingly similar to the phenomenology of resonance peaks in high-Tc and heavy fermion superconductors. The energy of the resonance peak scales with $T_{HO} \omega_{res} \sim 4 k_{BT_{HO}}$

1This work was supported by US DOE at LANL.
2:42PM D41.00002 Thermodynamical Properties across Quantum Critical Points...JIANDA WU, LIJUN ZHU, QIMIAO SI Quantum critical points (QCPs) are of extensive current interest, in part because they strongly influence the physical properties at finite temperatures. Thermodynamical properties have recently been used as a means to probe the energy scales in the quantum critical heavy fermion metals [1]. In addition, the divergence of the Gruneisen ratio (thermal expansion to specific heat) or its magnetic analog at any QCP, theoretically predicted a few years ago [2], has been observed in a growing list of quantum critical materials. In this work, we study the entropy as a function of control parameter in several theoretical models for quantum criticality. We explicitly demonstrate that the entropy is maximized near the QCP, which is compatible with the divergence of the Gruneisen ratio exactly at the QCP. When the control parameter is a magnetic field, we also study the field dependence of the isothermal magnetization and other magneto-thermal properties. [1] P. Gegenwart et al, Science 315, 969 (2007); [2] L. Zhu et al, PRL 91, 066404 (2003).

2:54PM D41.00003 Cyclotron Resonance in the Hidden-Order Phase of Ultraclean URu$_2$Si$_2$ Single Crystals... T. SHIBAUCHI, K. HASHIMOTO, K. IKADA, S. TONEGAWA, H. SHISHIDO, Department of Physics, Kyoto University, Y. HAGA, T. D. MATSUDA, Advanced Science Research Center, Japan Atomic Energy Agency, Y. ONUKI, Graduate School of Science, Osaka University, H. YAMAGAMI, Department of Physics, Kyoto Sangyo University, Y. MATSUDA, Department of Physics, Kyoto University — In the heavy fermion compound URu$_2$Si$_2$, the hidden-order transition occurs at 17.5 K, whose origin is still an enigma. Of primary importance is elucidating the electronic structure of the hidden-order phase. Here we report the first observation of cyclotron resonance in the ultraclean crystals of URu$_2$Si$_2$ with residual resistivity ratio $RRR > 670$. The magnetic-field dependence of the microwave surface impedance in the Azbel-Kern geometry shows clear cyclotron resonance lines whose width has characteristic temperature dependence consistent with the transport measurements. In addition to the bands which have been previously identified in the quantum oscillation measurements, we newly find the missing band with the heaviest mass, which can account for the large specific heat coefficient in the hidden-order phase of URu$_2$Si$_2$.

3:06PM D41.00004 Reconstruction of the Fermi Surface Deep inside the Hidden-Order Phase of Very Clean URu$_2$Si$_2$... Y. MATSUDA, H. SHISHIDO, T. SHIBAUCHI, K. HASHIMOTO, Department of Physics, Kyoto University, Y. HAGA, T.D. MATSUDA, Advanced Science Reserach Center, Japan Atomic Energy Agency, Y. ONUKI, Graduate School of Science, Osaka University, T. Sasaki, T. OIZUMI, N. KOBAYASHI, Institute for Materials Research, Tohoku University, Y. IMANAKA, National Institute for material Science — The nature of the hidden order (HO) phase in URu$_2$Si$_2$ is a long standing mystery in heavy-fermion physics. It has been shown that the HO phase is destroyed at $H_{\mathrm{c}} = 36$ T ($T = 0$) and several new phases appear above $H_{\mathrm{c}}$. Here we studied the low temperature/high field phase of very clean URu$_2$Si$_2$, single crystals ($RRR > 670$) by the transport properties. We find that the Hall resistivity jumps at $H_{\mathrm{c}} = 22$ T well inside the HO phase and new quantum oscillations appear at high fields starting slightly below $H_{\mathrm{c}}$. These results indicate a reconstruction of the Fermi surface and a possible phase transition well inside the HO phase. The present results provide strong evidence that the HO transition is described by an itinerant rather than a localized electron picture.

3:18PM D41.00005 Probing the Hidden Order in URu$_2$Si$_2$ by Impurity Doping... SEUNG-HO BAEK, Los Alamos National Laboratory, NICHOLAS CURRO, U. of California, Davis, M. GRAF, A. BALATSKY, ERIC BAUER, JASON COOLEY, JIM SMITH — URu$_2$Si$_2$ exhibits a clear broken symmetry ground state at 17.5 K, but the nature of the order parameter has not been determined for more than two decades. Motivated by the fact that Rh doping in this compound induces antiferromagnetism, indicating that the hidden order is closely related with the antiferromagnetism, we studied $^{29}$Si NMR with varying Rh concentration. This $^{29}$Si NMR study reveals that the antiferromagnetism arises from the local suppression of the hidden order by Rh doping. We propose that the antiferromagnetism emerges as a result of the local suppression of the hidden order yet only within the long range hidden order phase.

3:30PM D41.00006 Electronic structure model of the hidden order and Fermi surface gapping in URu$_2$Si$_2$... PETER OPPENEER, SAAD ELGAZZAR, JAN RUSZ, MICHIO-SUZUKI, Uppsala University, JOHN MYDOSH, University of Cologne — The hidden order (HO) in the heavy-fermion superconductor URu$_2$Si$_2$ has been studied for more than 20 years, without that the nature of this unusual phase could be uncovered. We present a microscopic explanation for the mechanism of the hidden order, on the basis of state-of-the-art electronic structure calculations. In particular, we show that our calculations explain very well all the known properties of the paramagnetic and large moment antiferromagnetic (LMAF) phases. Exploiting the known experimental equivalence between the Fermi surface properties of the LMAF and HO phases, we identify the Fermi surface “hot spots” where a Fermi surface instability is lifted through spontaneous symmetry breaking, causing a surprisingly large Fermi surface gapping. We quantify that symmetry breaking through collective modes of antiferromagnetic moment excitations can induce a substantial Fermi surface gapping that consistently explains the transport properties and entropy loss of the HO phase.

3:42PM D41.00007 Heavy Fermion and non-Fermi Liquid Properties vs Size: From the Micro to the Nano...G.R. STEWART, J.S. KIM, Physics/University of Florida, K. SAMWER, Physikalisches Institut, Universitäts-Göttingen — Y. Y. Chen et al. have studied nanoparticles of several systems, including CePt$_2$I$_3$. We report here the specific heat, C, down to 0.05 K and $\chi$ to 2 K as a function of size for several Ce- and U-heavy Fermion and non-Fermi liquid (nFl) systems, including UBe$_{13}$ and Rh-doped CeRu$_2$Si$_2$. Using dry sieves (for larger particles) and aqueous suspension/filtration techniques using Isopore filters (for smaller particles), size gradations from 45-53 $\mu$m (essentially bulk) down to 0.6-1.2 $\mu$m were studied. One goal was to study the evolution of nFl behavior versus decreasing size at a Quantum Critical Point, where the spatial extent of the fluctuations should become infinite, or at least larger than the particle at some size. Ce-systems showed the beginning of Kondo peak behavior in C below 3 $\mu$m, however it was still possible to determine the evolution of the intrinsic low temperature nFl C/T vs $\log$ T in Rh-doped CeRu$_2$Si$_2$ as a function of decreasing size to address this goal. The effect of size on superconductivity and $m^*$ in UBe$_{13}$ will also be discussed. [1] Y. Y. Chen et al., Phys. Rev. Lett. 98, 157206 (2007).

3:54PM D41.00008 Quantum criticality in the Bose-Fermi Kondo model and the quantum-to-classical mapping... STEFAN KIRCHNER, QIMIAO SI, Rice University — The Bose-Fermi Kondo model (BFKM) occurs as the effective quantum impurity model within the Extended Dynamical Mean Field Theory (EDMFT) for quantum critical heavy fermion metals. The quantum critical point (QCP) of the BFK is therefore related to the one in the Kondo lattice model, relevant low-energy model for heavy fermion compounds. There have been indications that the QCP of the BFKM cannot be described in terms of a local O(3)-symmetric $\phi^4$-theory as predicted by the quantum-to-classical mapping, but the issue remains to be settled. In this work we demonstrate that the quantum-to-classical mapping for the spin-isotropic SU(N) BFKM breaks down in a large N limit[1]. We also show that this feature is associated with the Berry phase term of the spin path integral and therefore persists for finite N[2]. We analyze the influence of this breakdown on the dynamic scaling properties of the Kondo lattice obtained through the EDMFT, and also discuss the connection of our results with those of the Ising-anisotropic BFKM. [1] L. Zhu, S. Kirchner, Q. Si and A. Georges, PRL 93, 267201 (2004). [2] S. Kirchner and Q. Si, arXiv:0808.2647 (2008).
4:06PM D41.00009 Thermal expansion and magnetostriction of the heavy fermion antiferromagnet YbAgGe. G.M. SCHMIEDESHOFF, A.W. LOUBSURY, S.J. TRACY, Occidental College, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory/Iowa State University — YbAgGe is a stoichiometric heavy fermion compound that exhibits antiferromagnetic order and field induced quantum criticality. We will discuss this behavior, and present a unified phase diagram of this compound in the T-H plane, in light of our recent thermal expansion and magnetostriction measurements. We find a remarkable agreement between thermodynamic, transport and microscopic measurements on this model system. Work at Occidental College was supported by the National Science Foundation under DMR-0704406. Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

4:18PM D41.00010 Magnetic-field-dependence of the YbRh$_2$Si$_2$ Fermi surface. PATRICK ROURKE, ALIX MCCOLLAM, University of Toronto, GERARD LAPIERT, GEORG KNEBEL, JACQUES FLOQUET, DFMPC, SPSMS, CEA Grenoble, STEPHEN JULIAN, University of Tokyo — Magnetic-field-induced changes of the Fermi surface play a central role in theories of the exotic quantum criticality of YbRh$_2$Si$_2$. We have carried out de Haas–van Alphen measurements in the magnetic field range 8 T $\leq H \leq 16$ T, and directly observe field-dependence of the extremal Fermi surface areas. Our data support the theory that a low-field “large” Fermi surface, including the Yb $4f$ quasi-hole, is increasingly spin-split until a majority-spin branch undergoes a Lifshitz transition and disappears at $H_d \approx 10$ T, without requiring $4f$-localization at $H_d$.

4:30PM D41.00011 Electron Spin Resonance in a Kondo lattice. PEDRO SCHLOTTMANN, Florida State University — Until recently it was commonly believed that due to the broad linewidth electron spin resonance (ESR) could not be observed in heavy-fermion compounds. This proven to be wrong, since an ESR signal was found in single crystals of YbRh$_2$Si$_2$ as well as in other systems. Recently, Abrahams and Wölfle$^1$ studied the ESR signal of a heavy fermion band within the framework of the Anderson lattice. They obtained that the heavy mass in conjunction with ferromagnetic fluctuations can lead to narrow resonances, and concluded that the observed ESR in YbRh$_2$Si$_2$ is due to the heavy fermion conduction states and not the Kondo localized moments. Here I study the ESR linewidth for localized moments within the framework of the Kondo lattice model. An ESR signal can only be observed if the Kondo temperature is sufficiently small. In addition, to obtain an observable signal short-range ferromagnetic correlations between the localized spins are necessary, which may lead to a bottleneck situation, that narrows the linewidth. It is concluded that from ESR data alone it is not possible to distinguish if the resonance is due to localized spins or conducting heavy electron spins. Work supported by the Department of Energy under grant No. DE-FG02-98ER45797.

4:42PM D41.00012 Crystalline Synthesis of Novel Yb-Pt-Pb Phases. CARLOS MARQUES, Brookhaven National Laboratory and Stony Brook University, YURI JANSSEN, Brookhaven National Laboratory, MARCUS BENNET, University of Michigan, MOO SUNG KIM, KEESOEONG PARK, Brookhaven National Laboratory, PETER KHALIFAH, MEIGAN ARONSON, Brookhaven National Laboratory and Stony Brook University — We have used flux techniques to explore the Yb-Pt-Pb ternary phase diagram, and have grown a number of intermetallic compounds including YbPt$_4$, Yb$_3$Pt$_5$, and the new Yb$_2$Pt$_9$, Yb$_3$Pt$_{10}$, Yb$_4$Pt$_{12}$, and Yb$_5$Pt$_{12}$Pb, as well as Yb$_2$Pt$_8$Si and Yb$_4$Pt$_8$Si. The crystal structure of these different compounds will be compared. A particular focus has been the synthesis of single crystals of quantum critical antiferromagnet (AF) Yb$_3$Pt$_4$, and we show that it is possible to synthesize crystals which are large enough for neutron diffraction measurements. Laue patterns and neutron rocking curves along with other methods show that these crystals are of very high quality. Initial results of neutron diffraction and inelastic scattering experiments on single Yb$_2$Pt$_9$ crystals and arrays of multiple Yb$_2$Pt$_9$ crystals will be presented.

$^1$Work at Stony Brook was supported by the National Science Foundation under grant NSF-DMR-0405961.

4:54PM D41.00013 Neutron scattering studies on Yb$_3$Pt$_4$. Y. JANSSEN, Brookhaven National Laboratory, M.C. BENNETT, Brookhaven National Laboratory and University of Michigan, C. MARQUES, L. WU, Brookhaven National Laboratory and Stony Brook University, M.S. KIM, K.S. PARK, Brookhaven National Laboratory, Q. HUANG, J.Y. LI, Y. CHEN, J.W. LYNN, NCNR NIST, M.C. ARONSON, Brookhaven National Laboratory and Stony Brook University — The antiferromagnetic (AF) intermetallic compound Yb$_3$Pt$_4$ shows a magnetic phase diagram which includes a quantum critical point, but is different from other Yb-containing quantum critical compounds. We elucidated the zero-field behavior by neutron scattering on both polycrystal and single-crystal samples. The magnetic structure due to the single-site-low-symmetry Yb moments was determined by diffraction. The AF unit cell coincides with the crystallographic unit cell, and shows pairs of Yb nearest-neighbor moments pointing directly towards each other. The order parameter is consistent with a continuous transition at the Néel temperature (2.4 K) and can be described by a simple mean-field model. The ordered moment amounts to $\sim 1.2 \mu_B$/Yb at 0 K. Inelastic neutron scattering reveals that the crystal electric field lifts the degeneracy of the Yb 4f ground state into 4 doublets, consistent with specific heat results.

$^3$This research is supported by NSF under grant NSF-DMR-0405961.

Monday, March 16, 2009 8:00PM - 9:12PM — Session G1 Energy and the Environment Spirit of Pittsburgh Ballroom A

8:00PM G1.00001 The flow of energy through the climate system and changes with global warming. KEVIN E. TRENBERTH, National Center for Atmospheric Research — A review is first given of the mean and annual cycle of energy flowing through the climate system, and its storage, release, and transport in the atmosphere, ocean, and land surface as estimated with recent observations. Of the roughly 175 Petawatts coming into the planet, about 120 are absorbed and drive the weather and climate system through the unequal distribution with latitude and between land and ocean. We are able to close the energy budget reasonably well, although largest errors are determined to be in changes in ocean heat content, especially south of about 35°S. The winter hemisphere atmospheric circulation is identified as the dominant contributor to poleward energy transports outside of the Tropics (6 to 7 PetaWatts), with summer transports being relatively weak ($\sim 3$ PW) slightly more in the Southern Hemisphere and slightly less in the Northern Hemisphere. Ocean transports outside of the Tropics are found to be small ($< 2$ PW) for all months. The current imbalance in radiation at the top-of-atmosphere (about 0.5 PW) owing to human-induced increases in greenhouse gases means that the atmosphere, land and ocean are warming up, and ice is melting, leading to a rise in sea level. This comes about from increasing greenhouse gases in the atmosphere, notably carbon dioxide, from human activities. The interference with the natural flows of energy is a factor of 60 or so larger than the direct energy released by human activities. A brief outline will be given of the resulting climate change underway and projections for the future.
8:36PM G1.00002 Materials for Sustainable Energy, GEORGE CRABTREE, Argonne National Laboratory — The global dependence on fossil fuels for energy is among the greatest challenges facing our economic, social and political future. The uncertainty in the cost and supply of oil threatens the global economy and energy security, the pollution of fossil combustion threatens human health, and the emission of greenhouse gases threatens global climate. Meeting the demand for double the current global energy use in the next 50 years without damaging our economy, security, environment or climate requires finding alternative sources of energy that are clean, abundant, accessible and sustainable. The transition to greater sustainability involves tapping unused energy flows such as sunlight and wind, producing electricity without carbon emissions from clean coal and high efficiency nuclear power plants, and using energy more efficiently in solid-state lighting, fuel cells and transportation based on plug-in hybrid and electric cars. Achieving these goals requires creating materials of increasing complexity and functionality to control the transformation of energy between light, electrons and chemical bonds. Challenges and opportunities for developing the complex materials and controlling the chemical changes that enable greater sustainability will be presented.

Tuesday, March 17, 2009 8:00AM - 11:00AM
Session H1 DCMP: Electronic Structure of Disordered Graphene Spirit of Pittsburgh Ballroom A

8:00AM H1.00001 Scanning Single Electron Transistor Microscopy on Graphene1, JENS MARTIN, Harvard University — We use a scanning single electron transistor to map the local density of states of graphene and the carrier density landscape in the vicinity of the neutrality point. At zero magnetic field our results confirm the existence of electron-hole puddles. These puddles could explain graphene’s anomalous non-zero minimal conductivity at zero average carrier density. Moreover, we find that, unlike non-relativistic particles the density of states can be quantitatively accounted for by considering non-interacting electrons and holes. At high magnetic field we investigate the appearance of localized states. Particle localization is an essential ingredient in quantum Hall physics. In conventional high mobility two-dimensional electron systems Coulomb interactions were shown to compete with disorder and to play a central role in particle localization. Surprisingly, despite the stronger disorder in graphene compared to the standard two-dimensional systems, our findings indicate that localization in graphene is also dominated by Coulomb interactions and not single particle physics.

1 in co-operation with J.Smet, MPI Stuttgart, Germany

8:36AM H1.00002 Magnetic Oscillations and Landau Quantization in Decoupled Epitaxial Graphene Multilayers*, JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 — A fundamental challenge to the development of a new electronics based on single atomic sheets of carbon, known as graphene, is to realize a large-area production platform that can produce a carbon system with the same intrinsic properties as a single sheet of graphene. Multi-layer epitaxial graphene (MEG) grown on SiC substrates has been proposed as a possible platform to this end [1]. The central question is, Can MEG behave as single layer graphene with the same intrinsic electrical characteristics? In this talk we show that MEG graphene on SiC exhibits single layer graphene properties through new tunneling magnetic measurements. The circular motion of electrons in a magnetic field has historically been a powerful probe of the Fermi surface properties of materials. Oscillations in many measurable properties, such as magnetization, thermal conductivity, and resistance, all reflect the Landau quantization of the electron energy levels. In this talk we show the ability to observe tunneling magneto-conductance oscillations (TMCOs) in the tunneling differential conductance as a function of both magnetic field and electron energy. The TMCO arise from intense Dirac quantization of the 2-dimensional Dirac electron and hole quasiparticles in MEG grown on SiC substrates. Spatial profiles of the Landau quantization demonstrate the high quality of MEG on SiC with carrier concentrations that vary less than 10% over hundreds of nm. The single layer quantization observed in these multi-layer samples is attributed to observed rotational stacking domains that effectively decouple the carbon layers in MEG on SiC, thereby yielding single layer graphene properties in a large area carbon production method. *In collaboration with Lee Miller, Kevin Kubista, Gregory M. Rutter, Ming Ruan, Mike Sprinkle, Claire Berger, Walt A. de Heer, and Phillip N. First, Georgia Institute of Technology

9:12AM H1.00003 Effect of potential barriers on transport in graphene1, B. HUARD, Physics Department, Stanford University, Stanford, CA 94025, USA — The energy of graphene charge carriers grows linearly with their momentum. This zero-mass behavior, associated with an absence of a forbidden region between electrons and holes, deeply modifies transport properties of electrons across potential steps and barriers. We perform transport measurements in graphene monolayers where the potential profile is tuned by a set of local gates [1,2]. By varying the height and width of potential barriers and the energy of charge carriers, we can test the predictions on the transmissions of the conduction channels across a potential step in graphene. Besides, we observe the effect of disorder and of screening of an external field in graphene. These experiments have a direct consequence in any transport measurement in graphene. We indeed showed that such potential steps naturally develop at the interface between graphene and a metallic electrode [3]. We discuss the effects of these steps in various geometries [4]. In collaboration with N. Stander, J.A. Sulpizio, Physics Department, Stanford University, Stanford, CA 94025, USA; and J. Cayssol, D. Goldhaber-Gordon, CPMOH, UMR5798, Université de Bordeaux, 33405 Talence, France.


1Present address : Laboratoire Pierre Aigrain, 24 rue Lhomond, 75005 Paris.
9:48AM H1.00004 Ground-state Properties of Inhomogeneous Graphene Sheets \textsuperscript{1}, MARCO POLINI, NEST-CNRS-IFM and Scuola Normale Superiore di Pisa — When inter-valley scattering is weak and gauge fields due to \textit{e.g.} ripples are neglected, doped and gated graphene sheets can be described using an envelope-function Hamiltonian with a new sublattice pseudospin degree-of-freedom, an ultrarelativistic massless-Dirac free-fermion term, a pseudospin \textit{scalar} disorder potential, and a non-relativistic instantaneous Coulombic interaction term. There is considerable evidence from experiment that this simplified description of a honeycomb lattice of Carbon atoms is usually a valid starting point for theories of those observables that depend solely on the electronic properties of \textit{n}-electrons near the graphene Dirac point [1]. Although the use of this model simplifies the physics considerably it still leaves us with a many-body problem without translational invariance, which we do not know how to solve. In this talk we present a Kohn-Sham-Dirac density-functional theory (DFT) scheme for graphene sheets that treats slowly-varying inhomogeneous scalar external potentials and electron-electron interactions on an equal footing [2]. The theory is able to account for the unusual property that the exchange-correlation contribution to chemical potential increases with carrier density in graphene [3,4]. Consequences of this property, and advantages and disadvantages of using the DFT approach to describe it, are discussed. The approach is illustrated by solving the Kohn-Sham-Dirac equations self-consistently for a model random potential describing charged-point-like impurities located close to the graphene plane. The influence of electron-electron interactions on these non-linear screening calculations is discussed at length, in the light of recent experiments [5,6] reporting evidence for the presence of electron-hole puddles in nearly-neutral graphene sheets.

\begin{thebibliography}{99}
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\textsuperscript{1}Work done in collaboration with Andrea Tomadin, Reza Asgari, and A.H. MacDonald. M.P. was supported by the CNR-INFM “Seed Projects”.

10:24AM H1.00005 Ground-state of Two-dimensional Graphene in the Presence of Random Charged Impurities \textsuperscript{1}, ENRICO ROSSI, Condensed Matter Theory Center, University of Maryland — The low energy electronic excitations of graphene are described by a massless Dirac fermion model. In clean isolated graphene the Fermi energy lies exactly at the Dirac point where the linear chiral electron and hole bands cross each other. Close to the Dirac point the average carrier density vanishes and the density fluctuations are expected to dominate the physics of graphene. In current experiment the fluctuations are mostly due to quenched disorder. In this talk I present the Thomas-Fermi-Dirac (TFD) theory [1] to calculate the \textit{carrier density} of graphene in presence of disorder. The TFD theory includes the effects of non-linear screening, exchange and correlation. The approach is independent of the disorder source and very efficient allowing the calculation of disorder-averaged quantities that can be directly compared with experiments. Recent transport results strongly suggest that in current graphene samples charge impurities are the main source of disorder. I then present the results of the TFD theory for this case. I show that close to the Dirac point the carrier density breaks up in electron-hole puddles and is characterized by two types of inhomogeneities: wide regions of low density and sparse narrow regions of high density and a typical correlation length of \textit{10 nm}. I present detailed results that show how the disordered averaged quantities characterizing the carrier density profile depend on the experimental parameters. I show that at finite voltages the density probability distribution has a bimodal character providing direct evidence for the existence of puddles over a finite range of gate voltages. In graphene the exchange-correlation term increases with density contrary to parabolic-band electron liquids and because of this it tends to suppress density inhomogeneities. I show that this effect becomes very important close to the Dirac point, especially at low impurity densities.

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Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H2 DPOLY: Polymer Physics Prize Symposium Honoring Steve Granick Spirit of Pittsburgh Ballroom BC

8:00AM H2.00001 Polymer Physics Prize Talk: Polymer Mobility at Surfaces and in Confined Environments, STEVE GRANICK, University of Illinois at Urbana-Champaign — Rich new chemistry and physics emerge when one considers confined fluids, where the environment is distinctly different than in bulk. The intuition of what to expect based on bulk properties is found to break down. This talk will emphasize recent findings using a combination of single-particle imaging and fluorescence correlation spectroscopy of polymers at hard surfaces (mica), soft surfaces (phospholipid bilayers) and random network environments. A surprising dependence is found on the polymer molecular weight and concentration, as well as on the substrate makeup.

8:36AM H2.00002 Engineered Colloids Having Particles of Controlled Size, Shape, and Chemistry \textsuperscript{1}, JOSEPH DESIMONE, UNC Chapel Hill — This lecture will focus on opportunities for complex particles made using a novel “top-down” fabrication method called PRINT (Particle Replication In Non-wetting Templates). PRINT enables the production of monodisperse, shape-specific nano and micro-particles from an extensive range of organic and inorganic liquid precursors. The assembly of colloidal particles has long been a rich and continuously growing area of materials science, with great potential for a broad range of applications including electronics, control systems, optics and biotechnology. Within this field, the bulk of research has been devoted to studying the assembly of isotropic spherical particles. In spite of this, there has been a growing interest in studying the assembly of anisotropic particles due to the more complex and useful structures that these particles can potentially assemble into. There are few reports on the assembly of anisotropic particles, in part because of the lack of effective fabrication processes for the preparation of these particles with the monodispersity, control and range of compositions required for in-depth study. Herein we will discuss the use of PRINT to fabricate monodisperse, nanometer- and micron-sized particles of varying size, shape and composition. PRINT stands out because of the high degree of molding resolution, the broad range of chemistries that can be molded, and the ease with which reel-to-reel technology can be incorporated for scalability. Thus, it is ideally suited to the synthesis of unique, highly anisotropic particles in a wide range of compositions. Herein we discuss the use of dielectrophoresis to study the assembly of highly anisotropic polymer particles: rods, discs, hexnuts and boomerangs, fabricated with the PRINT process. In addition, the discussion will focus on the details and opportunities for loading shape controlled particles with magnetite and their manipulation when dispersed in various liquid media.

\textsuperscript{1}Departments of Chemistry & Pharmacology, University of North Carolina at Chapel Hill; Dept. of Chemical & Biomolecular Engineering, North Carolina State University
9:12AM H2.00003 Polymers under Cylindrical Confinement, THOMAS RUSSELL, University of Massachusetts — Anodized alumina oxide (AAO) membranes offer a unique platform to investigate polymers under confinement. AAO membranes have been prepared where the diameters of the nanopores in the membrane have been varied from 8 to 50 nm by varying the anodization conditions. Capillary force is sufficiently large to draw high molecular weight polymers into the membrane, producing either nanotubes or nanorods. Polymer solutions can also be used place a thin film on the walls of the nanopores, forming nanotubes. With pore diameters less than the radius of gyration, a quantitative understanding of perturbations to chain dynamics due to geometric constraints was examined. We found a weak molecular weight-dependent mobility of polymers confined within AAO nanopores having diameters smaller than the dimension of the chains in the bulk. The measured mobility of polymers in the confined geometry was much higher than the mobility of the unconfined chain. Rayleigh instabilities in thin polymer films confined within nanoporous alumina membranes were also found where periodic undulations on the film surface were found to increase with time, eventually bridging across the cylindrical nanopore, resulting in the formation of polymer nanorods with a periodic array of encapsulated holes. We use microphase separated block copolymers, where the characteristic period of the BCP morphology is comparable to the pore diameter, significant deviations from the bulk morphology as revealed by electron tomography. Small angle neutron scattering was also used to investigate the influence of cylindrical confinement on the order-disordered transition. This work was done in collaboration with T. J. McCarthy (UMass), K. Shin (Seoul National University), H. Jinmai (Kyoto University), D. Chen, J. Chen, H. Xiang, T. Kim, and P. Dobryalov, and was supported by the DOE, NSF MRSEC, NSF CHM.

9:48AM H2.00004 The Challenge of Understanding the “Complexity” of Polymeric Fluids and Solutions, JACK DOUGLAS, Polymers Division, National Institute of Standards and Technology — It is well known that the complexity of polymer conformational shapes makes this class of molecules prone to glass formation and that high molecular mass polymers exhibit rubbery viscoelastic flow properties associated with their topological and packing interactions. Many natural and synthetic polymers also exhibit complex associative interactions arising from the variation of chemical species and the presence of charged and polar groups within the molecule that can give rise to polymer supermolecular organization into a wide range of fragile structures at the nanoscale and larger. There are changes in both the thermodynamics and dynamics of these fluids associated with these general patterns of “complex fluid” behavior that provide a fundamental challenge for theoretical understanding so that this field remains at the frontier of materials science. The high level of regularity observed in the relatively high frequency glassy dynamics of polymer fluids, and other glass forming liquids more broadly, and in the viscoelastic properties that define chain “entanglement” in high molecular mass polymers, provides some hope for a general theoretical framework describing the complex fluid dynamics of polymeric fluids. Specifically, it is argued, and supported by evidence, that the complex fluid behavior underlying glass formation, entanglement and self-assembly in polymeric fluids all involve emergent collective behavior taking the form of supermolecular polymer structures that form and disintegrate in dynamic equilibrium. This “dynamic heterogeneity” paradigm, which is not addressed by conventional mean field theories such as the mode-coupling model of glass formation and the reptation model, provides a framework for understanding many aspects of the linear and non-linear dynamics of polymer complex fluid behavior such as stretched exponential stress relaxation, and shear thinning and “aging” following cessation of flow. It also provides a framework for understanding the influence of nanoparticles, and other additives to polymeric fluids, that modify the fluid mesoscale structure, often with significant changes in material properties.

10:24AM H2.00005 Anisotropic Self-Assembly of Nanoparticle Amphiphiles, SANAT KUMAR, Columbia University — It is easy to understand the self-assembly of particles having anisotropic shapes or interactions, such as Co nanoparticles or proteins, into highly extended structures. However, there is no experimentally established strategy for creating anisotropic structures from common spherical nanoparticles. We demonstrate that spherical nanoparticles, uniformly grafted with macromolecules, robustly self-assemble into a range of anisotropic superstructures when they are dispersed in the corresponding homopolymer matrix. This phenomenon is driven by the microphase separation between the inorganic nanoparticles and the (organic) polymeric chains grafted to their surfaces in a fashion similar to block copolymers. This microphase separation driven particle self-assembly provides a unique means of controlling the global nanoparticle dispersion state in polymer nanocomposites. The relationship between the state of particle dispersion and nanocomposite properties can thus be critically examined, and in particular we focus on the mechanical reinforcement afforded when particles are added to polymers. Grafted nanoparticles are thus versatile building blocks for creating tunable and functional particle superstructures with significant practical applications. With Pinar Akcora, Hongjun Liu, Yu Li, Brian Benicewicz, Linda Schadler, Thanos Panagiotopoulos, Jack Douglas, P. Thiyagarajan and Ralph Colby.

1Supported by NSF-DMR.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H3 DBP: New Frontiers in Biomolecular Physics 301/302

8:00AM H3.00001 Are DNA transcription factor proteins Maxwellian Demons?, ALEXANDER YU. GROSBERG, New York University — This abstract is not available.

8:36AM H3.00002 The mechanism of load detection in the molecular motor myosin VI, ALEXANDER R. DUNN, Department of Biochemistry, Stanford University — Myosin VI is thought to act as both a molecular transporter and as an anchor in vivo. Recent results demonstrate that a rigid isolated alpha helix extends the myosin VI lever arm, generating an unexpectedly large stroke size of approximately 30 nm. Here we use single-molecule fluorescence, optical trapping, and gold nanoparticle tracking to examine the role of the lever arm extension in both myosin VI translocation and anchoring. Our results suggest that the rigidity of this unusual structural element plays an essential role in load-induced anchoring.

9:12AM H3.00003 Full Counting Statistics for Brownian Sieves and Brownian Molecular Machines, R. DEAN ASTUMIAN, University of Maine — A Brownian sieve is a spatially periodic microstructured device that combines the effects of thermal noise, local spatial asymmetry, and external forces to separate particles based on their transport properties. By treating the motion of an individual particle as a cyclical process in which the particle fluctuates away from and returns to the origin of some unit cell I derive generalized fluctuation-dissipation and reciprocal relations for the averages (for all moments) of the number of periodic displacements that are exact and valid for arbitrary values of the external forces. These relations hold not only for Brownian sieves, but for all molecular machines in which a nanoscale system couples two chemical, mechanical, or transport processes by a cycle in which the molecular machine itself fluctuates away from, and then returns to some arbitrary reference state, in the process doing or receiving work in an environment.

9:48AM H3.00004 Theory of protein misfolding and applications to misfolding diseases, STEVEN S. PLOTKIN, Department of Physics and Astronomy, University of British Columbia — Physics-based algorithms can predict the misfolding mechanisms of proteins involved in aggregation-related diseases, including ALS and the Prion diseases. Predictions based on such an algorithm that we have developed, which employs both atomistic interactions and surface-area based coarse-graining, have been recently verified by immunological assays and point to diagnostic and therapeutic applications. I will describe the results of our misfolding theory, and discuss future directions towards drug research.
10:24AM H3.00005 Theoretical methods for engineering protein structure and function. JEFFERY G. SAVEN, Department of Chemistry, University of Pennsylvania — Designing and engineering proteins provides ways to probe the determinants of folding, to facilitate their study, and to arrive at novel molecules, materials and nanostructures. Recent computational methods for identifying the properties of proteins consistent with a desired structure and function will be discussed. Computationally designed protein-based molecular systems will be presented, including proteins tailored to accommodate nonbiological cofactors and their novel functional properties.

Tuesday, March 17, 2009 8:00AM - 10:24AM –
Session H4 DCMP: New Developments in Heavy Electron Superconductivity 306/307

8:00AM H4.00001 New developments in our understanding of superconductivity in the 115 materials1, TUSON PARK, Los Alamos National Laboratory / Sungkyunkwan University — Is a quantum critical point (QCP) pertinent to unconventional superconductivity? There are several heavy-fermion compounds in which unconventional superconductivity emerges in proximity to a spin-density-type quantum-critical point (1). The absence of superconductivity in prime candidates for a local or Kondo-breakdown quantum criticality, however, raises the question of whether this type of criticality could benefit superconductivity (2). Using the heavy-fermion antiferromagnet CeRhIn5 as an example (3), we present the first evidence that critical modes associated with the Kondo-breakdown criticality can provide a new route to unconventional superconductivity. At a local QCP, accessed by applied pressure, magnetic and charge fluctuations coexist and produce electronic scattering that is maximal at the optimal pressure for unconventional superconductivity. References: (1) Mathur et al., Nature 394, 39 (1998); Monthoux et al., Nature 450, 1177 (2007). (2) Gegenwart et al., Nat. Phys. 4, 186 (2008). (3) T. Park et al., Nature 440, 65 (2006); T. Park et al. Proc. Nat. Acad. Sci. 105, 6825 (2008).

1Work at Los Alamos National Laboratory was performed under the auspices of the US Department of Energy, Office of Science.

8:36AM H4.00002 Unconventional superconductivity of NpPd5Al2, DAI AOKI, CEA-Grenoble — The 5f electrons in actinide compounds has an intermediate character between the 4f-localized state and the 3d-itinerant state. This leads to a variety of exotic phenomena, such as non-Fermi liquid behavior, multipole ordering, broken state order and unconventional superconductivity. The discovery of superconductivity in PuCoGa5 and PuRhGa5 with high critical temperatures provides a new perspective on the physics of actinides compounds. It is generally believed that Np compounds have more 5f-related character features like d-electron metals compared with U compounds. In fact, the results of dhYAs experiments in Np-115 compounds are in good agreement with the 5f-itinerant band model. However, the complicated magnetic properties in Np-115 are well explained by the mean field theory including the orbital ordering based on the 5f-localized model. This indicates the dual nature of 5f electrons. NpPd5Al2 is the first Np-based heavy fermion superconductor with the ZrNiAl-type tetragonal structure. The superconductivity was found below Tc = 5 K. The non-Fermi liquid behavior and the large specific heat coefficient (γ ≈ 200 mJ/K2mol) were detected. The upper critical field Hc2 at 0 K is large and highly anisotropic: 37 kOe for H || [100] and 143 kOe for H || [001]. Hc2 is strongly suppressed by the magnetic field in the Hc2–T phase diagram for both field direction, indicating the strong Pauli paramagnetic effect. The d-wave spin-singlet superconductivity is most likely realized. The large specific heat jump ΔC/γTc ≈ 2.33 suggests the superconductivity with strong coupling. The results are compared with the well known heavy fermion superconductor CeCoIn5.

9:12AM H4.00003 Heavy electrons and symplectic symmetry of a spin1, MAXIM DZEROTO, Rutgers University — Motivated by the recent discovery of the heavy fermion materials NpPd5Al2 [1] and PuCoGa5 [2] which transform directly from Curie paramagnets into superconductors, we have developed a novel theory of these materials based on the idea of composite pairing between local moments and electron pairs. This talk will discuss a simple model of this kind of pairing that can be solved exactly in a large-N limit [3]. The talk will discuss how this concept enables us to understand the giant entropy of condensation, the symmetry of the order parameter as well as an enhancement of the Andreev reflection in tunneling measurements and an upturn in the NMR relaxation rate above Tc. References: (1) Mathur et al., Nature 394, 39 (1998); Monthoux et al., Nature 450, 1177 (2007). (2) Gegenwart et al., Nat. Phys. 4, 186 (2008). (3) T. Park et al., Nature 440, 65 (2006); T. Park et al. Proc. Nat. Acad. Sci. 105, 6825 (2008).

1This work was funded by NSF grant DMR 0605935.

9:48AM H4.00004 Quantum Criticality and Superconductivity in β-YbAlB4, SATORU NAKATSUJI, University of Tokyo — Heavy fermion systems have provided a number of prototypical compounds to study unconventional superconductivity and non-Fermi-liquid (NFL) states. A long standing issue in the research of heavy fermion superconductivity in 4f intermetallics is the dramatically different behavior between the electron like Ce (4f1μ) and hole like Yb (4f11+) compounds. While superconductivity has been found in a number of Ce based heavy fermion compounds, no superconductivity has been reported for the corresponding Yb systems. In this talk, I present our recent finding of the superconductivity in the new heavy fermion system β-YbAlB4 [1–3]. The superconducting transition temperature is 80 mK, and above it, the system exhibits pronounced NFL behavior in the transport and thermodynamic properties [2,3]. Furthermore, the magnetic field dependence of the NFL behavior indicates that the system is a rare example of a pure metal that displays quantum criticality at ambient pressure and under zero magnetic field. Using our latest results, we discuss the detailed properties of superconductivity and quantum criticality. This is the work performed in collaboration with K. Kuga, Y. Matsumoto, T. Tomita, Y. Machida, T. Tayama, T. Sakakibara, Y. Karaki, H. Ishimoto, S. Yonezawa, Y. Maeno, E. Pearson, G. G. Lonzarich, L.Balicas, H. Lee, and Z. Fisk.

Tuesday, March 17, 2009 8:00AM - 11:00AM –
Session H5 FIAP FGSA: Physicists as Entrepreneurs 401/402

8:00AM H5.00001 From a PhD in Physics to Manufacturing Carbon Nanotubes, XINDI WU, C Nanotechnology — No abstract available.
8:36AM H5.00002 Building an R&D Based Company, R.D. VISPUTE, Blue Wave Semiconductors, Inc. — Entrepreneurship is the wellspring of innovation and the ability to seek out opportunities and turn them to profitable businesses. It is also closely associated with desire to succeed with taking risk. According to the U.S. Small Business Administration, entrepreneurs are major contributors to our economy. Entrepreneurs are also major employers, as small businesses generate 60-80 percent of all new jobs annually. It is agreed that small businesses are one of the key engines of economy and growth by contributing to employment creation. In this regard, having your own business is regarded as one of the most respectable pathways to prosperity and fulfillment. While some strike success the first time around, most successful entrepreneurs overcome several hurdles before succeeding. In my talk I will present my experience in starting my technology based company. “Blue Wave Semiconductors, Inc.” I will focus on opportunities as well as numerous factors faced as the small technology start-up including finance, access to Small Business Innovation Research (SBIR), identifying market, managerial skills, team and infrastructure development. Also, I will highlight some of the important factors such as perseverance, independence, ingenuity, confidence and the determination to overcome barriers for eventual success. If you are sitting on a great idea that can possibly create a good technology business and you don’t know where to start, then this talk will be helpful for getting your dream closer and resolving your risk factors for great rewards.

9:12AM H5.00003 Lessons Learned as a Serial Technology Entrepreneur, NICHOLAS ECONOMOU, Carl Zeiss SMT — Starting a new technology company can be an exciting experience, and can, on occasion, be financially lucrative as well. Aside from the obvious requirement to have some new technology to offer, the main impediment to making the leap is usually fear of unknown. This arises from several real issues: a) you don’t know how to do it; b) you assume the new situation will be less secure; c) you have to give up progress along your current career path; d) you fear failure itself, and how it will reflect on you as a person. There is no easy way to resolve these concerns, and although talking with others who have done it is helpful, the final decision is always difficult and very personal. Assuming you decide to go forward, there are some simple rules that will help along the way: 1. Have a PRODUCT idea, not just an innovative technology: it’s a business, not a way to continue interesting research. 2. Team up with experienced people in certain (not all) key jobs. The specifics depend on what your own skills are. 3. Make sure you have adequate funding at the outset to achieve some significant milestones. 4. Be selective about who funds you: they will be your business partners and will have a lot to say about what happens. 5. Start thinking about the liquidity/exit strategy from day one. The stories of how other companies were started and developed are good background information. Several of these from my own experiences will be discussed. They include a company that struggled for many years but ultimately went public and was successful, one that was quickly a success and was acquired, one that was an outright failure and two that continue on but with dubious prospects of success. Some thoughts on what went right or wrong, and what could have been done better will be presented.

9:48AM H5.00004 My experience with Bandwidth9, CONNIE CHANG-HASNAIN, University of California, Berkeley — No abstract available.

10:24AM H5.00005 The Roller Coaster Ride of an Entrepreneur, ZHIYUN CHEN, Pixelligent Technologies LLC — No abstract available.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H6 DCMP DAMOP: Quench Dynamics and Thermalization in Quantum Systems 406

8:00AM H6.00001 Eigenstate Thermalization Hypothesis and Quantum Thermodynamics1, MAXIM OLSHANII2, University of Massachusetts Boston — One of the open questions in quantum thermodynamics reads: how can linear quantum dynamics provide chaos necessary for thermalization of an isolated quantum system? To this end, we perform an ab initio numerical analysis of a system of hard-core bosons on a lattice and show [Marcos Rigol, Vanja Dunjko & Maxim Olsnianii, Nature 452, 854 (2008)] that the above controversy can be resolved via the Eigenstate Thermalization Hypothesis suggested independently by Deutsch [J. M. Deutsch, Phys. Rev. A 43, 2046 (1991)] and Srednicki [M. Srednicki, Phys. Rev. E 50, 888 (1994)]. According to this hypothesis, in quantum systems thermalization happens in each individual eigenstate of the system separately, but it is hidden initially by coherences between them. In course of the time evolution the thermal properties become revealed through (linear) decoherence that needs not to be chaotic.

1Supported by NSF and ONR.
2in collaboration with Marcos Rigol and Vanja Dunjko

8:36AM H6.00002 Microscopic diagonal entropy and many-body dynamics1, ROMAN BARANKOV, Boston University — We define microscopic diagonal entropy to characterize many-body dynamics of systems far from equilibrium. For the systems prepared initially in thermal equilibrium, it increases with time and is related to the heat generated in the dynamics. We illustrate our results with numerical simulations of a toy-BCS model.

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9:12AM H6.00003 Statistics of the Work done in a Quantum Quench, ALESSANDRO SILVA, Abdus Salam ICTP — The quantum quench, i.e. a rapid change in time of a control parameter of a quantum system, is the simplest paradigm of non-equilibrium process, completely analogous to a standard thermodynamic transformation. The dynamics following a quantum quench is particularly interesting in strongly correlated quantum systems, most prominently when the quench in performed across a quantum critical point. In this talk I will present a way to characterize the physics of quantum quenches by looking at the statistics of a basic thermodynamic variable: the work done on the system by changing its parameters [1]. I will first elucidate the relation between the probability distribution of the work, quantum Jarzynski equalities, and the Loschmidt echo, a quantity that emerges usually in the context of dephasing. Using this connection, I will then characterize the statistics of the work done on a Quantum Ising chain by quenching locally or globally the transverse field. I will then show that for global quenches the presence of a quantum critical point results in singularities of the moments of the distribution, while, for local quenches starting at criticality, the probability distribution itself displays an interesting edge singularity. The results of a similar analysis for other systems will be discussed.


9:48AM H6.00004 ABSTRACT WITHDRAWN —

10:24AM H6.00005 ABSTRACT WITHDRAWN —

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H7 DBP: Cellular Imaging at the Nanometer Scale 407
Depletion (STED) microscopy where the spot diameter follows states and transitions of the fluorescent marker to neutralize the limiting role of diffraction. The first viable concept of this kind was Stimulated Emission barrier in far-field fluorescence microscopy. To set the scene for future directions, I will show that all these concepts share a common strategy: exploiting selected microscopy, the 3D-imaging of the interior of (live) cells requires the use of focused visible light. I will discuss new developments of optical microscopy that numerical aperture of the lens and λ. Dep. of NanoBiophotonics — The resolution of a far-field optical microscopy is usually limited to d ≈ 414/415, W. E. MOERNER, Stanford University — In the two decades since the first optical detection and spectroscopy of a single molecule in a solid (Phys. Rev. Lett. 62, 2535 (1989)), much has been learned about the ability of single molecules to probe local nanoenvironments and individual behavior in biological and nonbiological materials in the absence of ensemble averaging that can obscure heterogeneity. The early years concentrated on high-resolution spectroscopy in solids, which provided observations of lifetime-limited spectra, optical saturation, spectral diffusion, optical switching, vibrational spectra, and magnetic resonance of a single molecular spin. In the mid-1990’s, much of the field moved to room temperature, where a wide variety of biophysical effects were subsequently explored, but it is worth noting that several features from the low-temperature studies have analogs at high temperature. For example, in our first studies of yellow-emitting variants of green fluorescent protein (EYFP) in the water-filled pores of a gel (Nature 388, 355 (1997)), optically induced switching of the emission was observed, a room-temperature analog of the earlier low-temperature behavior. Because each single fluorophore acts a light source roughly 1 nm in size, microscopic imaging of individual fluorophores leads naturally to superresolution, or determination of the position of the molecule with precision beyond the optical diffraction limit (i.e., by discrimination of the point-spread function from the single emitter). Recent work has allowed measurement of the shape of single filaments in a living cell simply by allowing a single molecule to move through the filament (PNAS 103, 10929 (2006)). The additional use of photoswitched control of single-molecule emission allows imaging beyond the diffraction limit (superresolution) by several novel approaches proposed by different researchers. For example, using photoswitchable EYFP, a novel protein superstructure can now be directly imaged in a living bacterial cell at sub-40nm resolution (Nat. Meth. 5, 947 (2008)). These important advances provide the impetus for the further development of both new imaging schemes with 3-D capability as well as invention of new photoswitchable single-molecule emitters for use in polymers and in biological systems (JACS 130, 9204 (2008); J. Phys. Chem. B 112, 11878 (2008)).

Depletion (STED) microscopy where the spot diameter follows d ≈ 414/415, STEFAN HELL, Max Planck Institute for Biophysical Chemistry/Dep. of NanoBiophotonics — The resolution of a far-field optical microscopy is usually limited to d = λ/(2n sin α) ≈ 200 nm, with n sin α denoting the numerical aperture of the lens and λ the wavelength of light. While the diffraction barrier has prompted the invention of electron, scanning probe, and x-ray microscopy, the 3D-imaging of the interior of (live) cells requires the use of focused visible light. I will discuss new developments of optical microscopy that I anticipate to have a lasting impact on our understanding of living matter. Emphasis will be placed on physical concepts that have overcome the diffraction barrier in far-field fluorescence microscopy. To set the scene for future directions, I will show that all these concepts share a common strategy: exploiting selected states and transitions of the fluorescent marker to neutralize the limiting role of diffraction. The first viable concept of this kind was Stimulated Emission Depletion (STED) microscopy where the spot diameter follows d ≈ λ/(2n sin α(1 + I/I0)), I/I0 is a measure of the strength with which the molecule is send from the fluorescent state to the dark ground state. For I/I0 → ∞ it follows that d → 0, meaning that the resolution that can, in principle, be molecular. The concept underlying STED microscopy can be expanded by employing other transitions that shuffle the molecule between a dark and a bright state, such as (i) shelving the fluorophore in a dark triplet state, and (ii) photoswitching between a ‘fluorescence activated’ and a ‘fluorescence deactivated’ conformational state. Examples for the latter include photochromic organic compounds, and fluorescent proteins which undergo a cis-trans photoisomerizations. Photoswitching provides ultrahigh resolution at ultralow light levels. Switching can be performed in an ensemble or individually in which case the image is assembled molecule by molecule at high resolution. By providing molecular markers with the appropriate transitions, synthetic organic chemistry and protein biotechnology plays a key role in this endeavor. Besides being a fascinating development in physics, far-field optical “nanoscopy” is highly relevant to the life sciences. In fact, it has already been a key to answering important questions in biology [1, 2]. Due to its simplicity and improving performance, I expect far-field optical nanoscopy to enter virtually every cell biology laboratory in the near future.

References:
Formation, GEOFFREY POORE, Department of Physics, University of Illinois at Urbana-Champaign, SUSAN KIEFFER, Department of Geology, sensitive to these initial conditions, while the Hack exponent and hypsometry show little or no sensitivity. The results suggest that initial conditions deserve systematically studied. We used simulations of a stream power law, with initial conditions consisting of a flat or sloping surface combined with random dynamics. Previous research suggests that river network scaling and geomorphic properties may be sensitive to initial conditions, but this has not been.

2 normal diffusion to superdiffusion. That reaction fronts in this system typically pin to moving vortices. We explore any changes in front propagation behavior when the transport changes from forcing protocol. We find that the network with the oscillatory reaction synchronizes if the mixing is superdiffusive with long-range connections. We also find networks of branching angle and branching ratio for up to 10 branching generations. Both optimal angle and optimal ratios are found to be decreasing functions of or minimize expenditure of energy for different fixed numbers of absorbers. For constant salinity absorbers, we give the total water production rate as functions of having the same pressure difference across the absorbers, ii) all nodes producing permeate at identical rates, and iii) each node having the same salinity. Optimal criteria. Using the analogy to electrostatics, the diffusion equation is solved for the desalination systems under three different boundary conditions, i) all nodes introduced as Iterated Function Systems (IFS) to optimally design networks for efficient reverse osmosis desalination in deep seawater. Ramified flow networks and synchronization in an advection-reaction-diffusion system. The reaction is either the excitable or oscillatory Belousov-Zhabotinsky chemical reaction, and the flows is an array of annular chain of vortices forced using magnetohydrodynamic techniques. The reaction in each vortex acts as a node in a complex fluid network, and communication between these nodes is via chaotic mixing. Mixing in this system is either diffusive (enhanced) or superdiffusive, depending on the forcing protocol. We find that the network with the oscillatory reaction synchronizes if the mixing is superdiffusive with long-range connections. We also find that reaction fronts in this system typically pin to moving vortices. We explore any changes in front propagation behavior when the transport changes from normal diffusion to superdiffusion.

8:00AM H8.00001 Devastation and Renewal: Water, Air and Land in Pittsburgh Environmental History, JOEL TARR, Carnegie Mellon University — This talk will focus on the metabolism of cities as a concept through which to view the environmental history of Pittsburgh. In many ways, the history of Pittsburgh, perhaps more than that of any other city in the nation, reflects the impact of industrialism and of urban infrastructure on environmental quality. The talk will explore these effects and attempts at remediation through a slide lecture that will examine three domains: water supply and wastewater disposal; smoke and air pollution; and land contamination.

8:36AM H8.00002 Air Quality from Early Pittsburgh to the Present: The Science of Change, CLIFF DAVIDSON, Carnegie Mellon University — Throughout Pittsburgh's history over the past 250 years, coal reserves in the city and nearby have influenced its economy, demographics, and environmental quality. They have also played a major role in determining air quality in the region. For example, Pittsburgh became famous for its high particle loadings as early as the beginning of the nineteenth century, when the first complaints about air quality in the city were recorded. Nevertheless, residents tolerated the high coal smoke levels since jobs depended on the iron works, steel mills, and other industries. When natural gas was discovered just east of the city in the 1870's and replaced coal for some applications, particle concentrations decreased. But the local supplies of natural gas ran short several years later, and as industry continued to expand in the 1890’s the city went back to the use of coal as its primary fuel. The return to smoky air was met with resistance that marked the beginning of sustained public outcry and initiation of several air pollution studies. The next half century was marked by periods of occasional high and low concentration, the latter due to events such as the financial panic of 1907 and the depression of the 1930’s. It was not until the 1940’s that effective regulations were passed to reduce smoky conditions. Particle levels fell throughout the 1950’s and 1960’s, and eventually the decline of heavy industry in Pittsburgh led to relatively clean air in many parts of the city. Over the past few decades, airborne particle concentrations averaged across the Pittsburgh region have remained below their earlier levels. However, there are still "hot spots" of high concentration resulting from regional background coming from upwind areas and emissions of some large sources that have continued to operate in the Pittsburgh region. Furthermore, the composition of airborne particles in the city has changed from earlier times. Such particles are now the result of emissions from sources in upwind states, greater numbers of mobile sources, and the influence of control technologies that remove certain classes of pollutants but not others.

9:12AM H8.00003 Material Science and Construction, ALAN TRAUGOTT, CLJ Engineering — We will review the new materials and technologies that are being applied in the construction of high performance (green) buildings to improve energy efficiency, Indoor Air and Environmental Quality, water conservation and reclamation, and resource conservation. We present an introduction to state-of-the-art building concepts, including “Net-Zero” buildings, which generate as much energy as they use, reclaim water, and minimize waste; and “Waste as Resource,” including waste to energy plants, biofuels, materials reclamation and recycling. The role of advanced materials and technologies, such as spectrally selective glazing, photocatalytic concrete, solar heating and cooling, and organic solar collectors will be discussed. We also give an overview of advanced analytic tools used in building design, including Computational Fluid Dynamics, energy, and lighting/daylighting computer-based simulation programs.

9:48AM H8.00004 The Greening of the David L. Lawrence Pittsburgh Convention Center, MARK LEAHY, The Lawrence Convention Center — The David L. Lawrence Convention Center is the largest Gold LEED NC (new construction) certified convention center in the USA and the first of its kind in the world. The designation has been awarded by the United States Green Building Council through its Leadership in Energy and Environmental Design (LEED) Green Building Rating System. In this talk we discuss the unique green properties of this 1.5 million square foot Convention Center including the design and use of daylight, natural ventilation and other sustainable design and practices. No other building the size of the Convention Center (1.5 million square feet), uses natural ventilation or can illuminate an exhibition hall entirely through its windows and skylights. Approximately 75% of the convention center’s exhibition space is lit by natural daylight. The use of natural ventilation and extensive day lighting is designed to reduce energy consumption by nearly 35% compared to traditional ventilated and lit buildings of a similar size.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H9 GSNP: Complex Networks and Their Applications 303

8:00AM H9.00001 Dependence on Initial Conditions in a Numerical Model of River Network Formation, GEOFFREY POORE, Department of Physics, University of Illinois at Urbana-Champaign, SUSAN KIEFFER, Department of Geology, University of Illinois at Urbana-Champaign — We investigated the effect of initial conditions on river network formation, using a simple model of erosional dynamics. Previous research suggests that river network scaling and geomorphic properties may be sensitive to initial conditions, but this has not been systematically studied. We used simulations of a stream power law, with initial conditions consisting of a flat or sloping surface combined with random fluctuations in elevation, and considered dependence of steady-state solutions on initial slope and randomness. The sinuosity exponent and the sinuosity are sensitive to these initial conditions, while the Hack exponent and hypsometry show little or no sensitivity. The results suggest that initial conditions deserve greater consideration in attempts to understand the emergence of scaling in river networks.

8:12AM H9.00002 Optimization of Ramified Flow Networks, MARTIN SINGLETON, ALFRED HUBLER, Department of Physics, UIUC, GREGOR HEISS, Institut fuer physikalische Chemie, Ludwig Maximilians Universitaet Muenchen — A class of Ramified graphs (RG) is introduced as Iterated Function Systems (IFS) to optimally design networks for efficient reverse osmosis desalination in deep seawater. Ramified flow networks of absorbers, ranging from simple structures with constant weights, branch angles, and branch ratios, to fully optimized binary networks are considered. A contracting IFS with fixed overall length is presented for the generation of RG’s which serve as candidates for optimality in terms of desalination performance criteria. Using the analogy to electrostatics, the diffusion equation is solved for the desalination systems under three different boundary conditions, i) all nodes having the same pressure difference across the absorbers, ii) all nodes producing permeate at identical rates, and iii) each node having the same salinity. Optimal branching angles and branch length ratios will be found by phase-space methods for each boundary condition, which either maximize production of permeate or minimize expenditure of energy for different fixed numbers of absorbers. For constant salinity absorbers, we give the total water production rate as functions of branching angle and branching ratio for up to 10 branching generations. Both optimal angle and optimal ratios are found to be decreasing functions of generation for constant salinity absorbers.

8:24AM H9.00003 Reaction fronts and synchronization in ordered and disordered vortex networks, TOM SOLOMON, GARRETT O’MALLEY, JUSTIN WINOKUR, Bucknell University — We present experimental studies of front propagation and synchronization in an advection-reaction-diffusion system. The reaction is either the excitable or oscillatory Belousov-Zhabotinsky chemical reaction, and the flows is an array of annular chain of vortices forced using magnetohydrodynamic techniques. The reaction in each vortex acts as a node in a complex fluid network, and communication between these nodes is via chaotic mixing. Mixing in this system is either diffusive (enhanced) or superdiffusive, depending on the forcing protocol. We find that the network with the oscillatory reaction synchronizes if the mixing is superdiffusive with long-range connections. We also find that reaction fronts in this system typically pin to moving vortices. We explore any changes in front propagation behavior when the transport changes from normal diffusion to superdiffusion.

1Supported by NSF Grants DMR-0703635 and PHY-0552790.
2Current address: Dept. of Physics, Carnegie-Mellon University
for evaluating the link partitions is also introduced. As a set of (related) links. We show how this alternative viewpoint incorporates significant aspects including overlapping communities. A quantitative framework for the problem of community detection in complex networks. Rather than defining a community as a set of densely interconnected nodes, we define a community as a family of novel fat-tail random matrix ensembles characterized by a parameter \( \lambda \). We show that the eigenvalue spectrum can be used as a tool to detect SD in real-life networks. We illustrate this ability for the eigenvalue spectrum of a spatially dependent polymeric gel.

A family of fat-tail random matrix ensemble, JIMMY CHO, K.A. MUTTALIB — We present a family of novel fat-tail random matrix ensembles characterized by a parameter \( \lambda \). We show that the eigenvalue densities of the ensembles exhibit a power law distribution. In particular, for \( \lambda > 1 \), the tail of the distribution is bounded, whereas for \( \lambda < 1 \), the distribution has a fat tail. In the limit \( \lambda = 1 \), the ensembles reduce to the GOE and critical ensemble. We evaluate the eigenvalue correlations in terms of a novel family of orthogonal polynomials that are generalizations of the q-Hermite polynomials. We show that the two-level correlation of the novel fat-tail ensemble is qualitatively different from that of either the Gaussian or the critical ensemble.

Poisson vaccination for epidemic control in adaptive social networks, LEAH SHAW, College of William and Mary, IRA SCHWARTZ, Naval Research Laboratory — We study an epidemic model for disease spread on an adaptive network modeling avoidance behavior. Individuals are assumed to adapt their social behavior to minimize their risk of disease. Non-infected nodes rewire their connections away from infected nodes to connect instead to other non-infected nodes, and the disease follows an SIS (susceptible-infected-susceptible) dynamics. We add Poisson distributed vaccination of susceptibles. Effects of the vaccination frequency and amplitude are studied in the full system and compared to a mean field theory. Disease extinction rates using vaccination are found for both adaptive and static networks. We show that vaccine control is much more effective in adaptive networks than in static networks due to an interaction between the rates of adaptive network rewiring and vaccine application.

Epidemics in Complex Networks: The Diversity of Hubs, MAKSIM KITSK, Boston University, LAZAROS K. GALLOS, The City College of New York, SHLOMO HAVLIN, Bar-Ilan University, H. EUGENE STANLEY, Boston University, HERNAN A. MAKSE, The City College of New York — Many complex systems are believed to be vulnerable to spread of viruses and information owing to their high level of interconnectivity. Even viruses of low contagiousness easily proliferate the Internet. Rumors, fads, and innovation ideas are prone to efficient spreading in various social systems. Another commonly accepted standpoint is the importance of the most connected elements (hubs) in the spreading processes. We address following questions. Do hubs conduct epidemics in the same manner? How does the epidemics spread depend on the structure of the network? What is the most efficient way to spread information over the system? We analyze several large-scale systems in the framework of of the susceptible-infected-susceptible (SIR) disease spread model which can also be mapped to the problem of rumor or fad spreading. We show that hubs are often ineffective in the transmission of virus or information owing to the highly heterogeneous topology of most networks. We also propose a new tool to evaluate the efficiency of nodes in spreading virus or information.

Prevalence of and Epidemic Spreading on Hierarchical Networks, JIANKUI HE, Department of Physics & Astronomy, Rice University, Houston, TX, 77005, USA, MICHAEL DEEM, Department of Physics & Astronomy, Department of Bioengineering, Rice University, Houston, TX, 77005, USA, MICHAEL W. DEEM TEAM — Recent studies show that real networks are organized in a modular or even hierarchical fashion. However, there is no clear mathematical definition of hierarchy and current studies do not tell us the degree to which a network is hierarchical. In this talk, we will discuss a quantitative measurement of hierarchy. We find that networks of protein interactions, metabolic pathways, electronic circuits, power grids, and email display strong hierarchy compared with networks generated at random or scale free networks of the Barabasi-Albert model. Further, we investigated the spread of virus in hierarchical networks. Viral spread on hierarchical networks displays quite different pattern from scale free and random networks.

Understanding the spreading patterns of mobile phone viruses, PU WANG, MARTA GONZALEZ, CESAR HIDALGO, ALBERT-LASZLO BARABASI — Mobile viruses are little more than a nuisance today, but given our increased reliance on wireless communication, in the near future they could pose more risk than their PC based counterparts. Despite of the more than three hundred mobile viruses known so far, little is known about their spreading pattern, partly due to a lack of data on the communication and travel patterns of mobile phone users. Starting from the traffic and the communication pattern of six million mobile phone users, we model the vulnerability of mobile communications against potential virus outbreaks. We show that viruses exploiting Bluetooth and multimedia messaging services (MMS) follow markedly different spreading patterns. The Bluetooth virus can reach all susceptible handsets, but spreads relatively slowly, as its spread is driven by human mobility. In contrast, an MMS virus can spread rapidly, but because the underlying social network is fragmented, it can reach only a small fraction of all susceptible users. This difference affects both their spreading rate, the number of infected users, as well as the defense measures one needs to take to protect the system against potential viral outbreaks.

Partitioning Links: A New Approach to Communities in Complex Networks, JAMES BAGROW, YONG-YEOL AHN, SUNE LEHMANN, ALBERT-LASZLO BARABASI, Northeastern University — We propose a new viewpoint for the problem of community detection in complex networks. Rather than defining a community as a set of densely interconnected nodes, we define a community as a set of (related) links. We show how this alternative viewpoint incorporates significant aspects including overlapping communities. A quantitative framework for evaluating the link partitions is also introduced.
analysis of their localization both in the $z$ and $(\text{In},\text{Ga})\text{As}$ quantum dots, using a multi-band atomistic pseudopotential approach. We offer a classification of both hole and electron states based on an approximation.

exhibit a large oscillator strength in optical absorption. We calculate oscillator strengths for various optical transitions in the framework of the effective mass paradox according to which some of the optical transitions in PbSe and PbS semiconductor nanocrystals seemingly forbidden by the parity selection rule.

tals: Drastic effect of structure inversion asymmetry, SERGUEI GOUPALOV

The observation of biexciton Stokes shift underpins the physics of optical gain in quantum dots. We report on the first observation of a biexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and biexciton fine structure. The spectrum of the biexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of spectrum of states of the biexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems. We report on the first observation of a biexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and biexciton fine structure. The observation of biexciton Stokes shift underpins the physics of optical gain in quantum dots.

The speed at which information travels from one site to another in a complex system is largely determined by the number of short-cuts within the network topology. It remains an important open question how to optimize the connectivity of the links in the network structure to minimize the travel time. Here we show that ideas taken from renormalization group theory applied to complex self-similar networks are essential to define distinct regimes of information flow within the network. We find that networks that are human decision based such as the WWW are sufficiently randomized to give a topology that is close to optimal. On the other hand, biological evolution-based networks show evidence of clear sign of a modular deterministic structure shaped by evolution showing suboptimal large-world character which may be even so as a mean of protection, preservation and conservation.


ditmate to understanding the physics of quantum dots. Patanjali Kambham-Pati, Samuel Sewall, Ryan Cooney, McGill University — Confinement of carriers in quantum dots results in hydrogenic like states for the exciton. Thus a single excitation in a quantum dot bears resemblance to a hydrogen atom; these materials are often referred to as “artificial atoms.” A pair of excitons will form a four body bexciton, akin to a helium atom. The excitonic $^2$He atom should have an eigenstate spectrum in the $\text{He}$ atomic orbitals. The eigenstate spectrum of the bexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of spectrum of states of the bexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems. We report on the first observation of a bexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and bexciton fine structure. The observation of bexciton Stokes shift underpins the physics of optical gain in quantum dots.

Coherent Optical Phenomena in Quantum Dots, DUNCAN G. STEEL, University of Michigan — The quantum confinement provided by a semiconductor quantum dot suppresses much of the many body physics associated with the coherent nonlinear optical response observed in higher dimensional systems. This makes them attractive for potential device applications where atomic like properties, such as high $Q$ resonances, strong optical interactions, or long quantum coherence times, could be important. In this talk, we present recent results demonstrating high field effects beyond Rabi oscillations including the Mollow absorption spectrum showing gain without inversion, dark state formation in single electron doped dots, and suppression of nuclear fluctuations by the hyperfine interaction leading to longer electron spin coherence times.

Creating an artificial periodic table using quantum dots, PATANJALI KAMHBAM-PATI, SAMUEL SEWALL, RYAN COONEY, McGill University — Confinement of carriers in quantum dots results in hydrogenic like states for the exciton. Thus a single excitation in a quantum dot bears resemblance to a hydrogen atom; these materials are often referred to as “artificial atoms.” A pair of excitons will form a four body bexciton, akin to a helium atom. The excitonic $^2$He atom should have an eigenstate spectrum in the $\text{He}$ atomic orbitals. The eigenstate spectrum of the bexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of spectrum of states of the bexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems. We report on the first observation of a bexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and bexciton fine structure. The observation of bexciton Stokes shift underpins the physics of optical gain in quantum dots.

Creating an artificial periodic table using quantum dots, PATANJALI KAMHBAM-PATI, SAMUEL SEWALL, RYAN COONEY, McGill University — Confinement of carriers in quantum dots results in hydrogenic like states for the exciton. Thus a single excitation in a quantum dot bears resemblance to a hydrogen atom; these materials are often referred to as “artificial atoms.” A pair of excitons will form a four body bexciton, akin to a helium atom. The excitonic $^2$He atom should have an eigenstate spectrum in the $\text{He}$ atomic orbitals. The eigenstate spectrum of the bexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of spectrum of states of the bexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems. We report on the first observation of a bexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and bexciton fine structure. The observation of bexciton Stokes shift underpins the physics of optical gain in quantum dots.

Drastic effect of structure inversion asymmetry, SERGUEI GOUPALOV, Jackson State University — We resolve a paradox according to which some of the optical transitions in PbSe and PbS semiconductor nanocrystals seemingly forbidden by the parity selection rule exhibit a large oscillator strength in optical absorption. We calculate oscillator strengths for various optical transitions in the framework of the effective mass approximation.

Attractive properties of localized resonances above the continuum in quantum dots, SERGUEI GOUPALOV, Jackson State University — We resolve a paradox according to which some of the optical transitions in PbSe and PbS semiconductor nanocrystals seemingly forbidden by the parity selection rule exhibit a large oscillator strength in optical absorption. We calculate oscillator strengths for various optical transitions in the framework of the effective mass approximation.

1 NSF-HSD

Renormalization describes distinct regimes of information flow in complex networks, HERNAN ROZENFELD, City College of New York, CHAOMING SONG, Northeastern University, HERNAN MAKSE, City College of New York — The speed at which information travels from one site to another in a complex system is largely determined by the number of short-cuts within the network topology. It remains an important open question how to optimize the connectivity of the links in the network structure to minimize the travel time. Here we show that ideas taken from renormalization group theory applied to complex self-similar networks are essential to define distinct regimes of information flow within the network. We find that networks that are human decision based such as the WWW are sufficiently randomized to give a topology that is close to optimal. On the other hand, biological evolution-based networks show evidence of clear sign of a modular deterministic structure shaped by evolution showing suboptimal large-world character which may be even so as a mean of protection, preservation and conservation.

1 NSF-HSD

Patterns of behavior in an online community, LAZAROS GALLOS, Levich Institute, City College of New York, DIEGO RYBSTKI, FREDRIK LILJEROS, SHLOMO HAVLIN, HERNAN MAKSE — Human behavior can be seen as the expression of inherent motives. Despite the diverse range of these motives, social theorists have long identified a small number of distinct underlying mechanisms, where, consciously or unconsciously, every individual tries to exploit a different aspect of social interactions and/or optimize the efficiency of certain procedures for the benefit of the society or for personal gain. Here we show that users in an online community follow certain behavioral patterns and the choice of their favorite members is far from a random process. More importantly, these patterns are systematically modified with time as a member becomes more involved in such a community. We are able to identify a crossover in the average behavior of the members when their favorites list exceeds roughly 10 favorites. Additionally, this process allows us to identify individuals with a markedly different behavior than the average person. This study can help us understand the process of establishing friendships and the motives behind this process.

Tuesday, March 17, 2009 8:00AM - 11:00AM
Session H10 DCMP: Focus Session: Optical Properties of Nanostructures I: Quantum Dots

Coherent Optical Phenomena in Quantum Dots, DUNCAN G. STEEL, University of Michigan — The quantum confinement provided by a semiconductor quantum dot suppresses much of the many body physics associated with the coherent nonlinear optical response observed in higher dimensional systems. This makes them attractive for potential device applications where atomic like properties, such as high $Q$ resonances, strong optical interactions, or long quantum coherence times, could be important. In this talk, we present recent results demonstrating high field effects beyond Rabi oscillations including the Mollow absorption spectrum showing gain without inversion, dark state formation in single electron doped dots, and suppression of nuclear fluctuations by the hyperfine interaction leading to longer electron spin coherence times.

Creating an artificial periodic table using quantum dots, PATANJALI KAMHBAM-PATI, SAMUEL SEWALL, RYAN COONEY, McGill University — Confinement of carriers in quantum dots results in hydrogenic like states for the exciton. Thus a single excitation in a quantum dot bears resemblance to a hydrogen atom; these materials are often referred to as “artificial atoms.” A pair of excitons will form a four body bexciton, akin to a helium atom. The excitonic $^2$He atom should have an eigenstate spectrum in the $\text{He}$ atomic orbitals. The eigenstate spectrum of the bexciton has remained elusive due to the ultrafast timescale of relaxation processes in quantum dots which mask observation of the excited states. Here, we show the first, direct observation of spectrum of states of the bexciton, completing the analogy of excitons in quantum dots to atomic and molecular systems. We report on the first observation of a bexciton Stokes shift, which we will discuss in terms of non-Aufbau filling and bexciton fine structure. The observation of bexciton Stokes shift underpins the physics of optical gain in quantum dots.

Selection rules for optical transitions in lead salts semiconductor nanocrystals: Drastic effect of structure inversion asymmetry, SERGUEI GOUPALOV, Jackson State University — We resolve a paradox according to which some of the optical transitions in PbSe and PbS semiconductor nanocrystals seemingly forbidden by the parity selection rule exhibit a large oscillator strength in optical absorption. We calculate oscillator strengths for various optical transitions in the framework of the effective mass approximation.

1 Also at A.F. Ioffe Physico-Technical Institute, Russian Academy of Sciences

The appearance of localized resonances above the continuum in quantum dots, VOICU POPESCU, National Renewable Energy Lab, Golden CO, GABRIEL BESTER, Max Planck Institute for Solid State Research, Stuttgart, Germany, ALEX ZUNGER, National Renewable Energy Lab, Golden CO — We investigate the nature of hole and electron states in self-assembled InAs/GaAs and (In,Ga)As quantum dots, using a multi-band atomistic pseudopotential approach. We offer a classification of both hole and electron states based on an analysis of their localization both in the $z$ and $xy$-directions. We show that the coherent dot-matrix strain present in self-assembled quantum dots distorts the electron confining potential, creating "wings" in the vicinity of the dot. This results in the appearance of dot-confined electronic states that lie above the continuum of the matrix material. The spectroscopic manifestation of these resonant states is investigated, by calculating the inter-band as well as the intra-band absorption spectra. We find, in both cases, that clear finger-prints of the resonances appear, in the form of sharp, well-defined peaks. In contrast, the previously suggested "cross-transitions" between wetting-layer states and dot states are shown to disappear once realistic strain is included.

1 Funded by DOE-SC-BES-MSED through NREL Contract DE-AC36-08GO28308.
9:12AM H10.00005 Effect of Atomic-Scale Alloy Randomness on the Optical Polarization of Semiconductor Quantum Dots\textsuperscript{1}. VLAGAN MLINAR, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — Alloyed Ga\textsubscript{x} In\textsubscript{1-x} As system consists of different random assignments \( \sigma \) of the Ga and In atoms to the cation sublattice sites; each configuration having, in principle, distinct physical properties. For self-assembled dots made of finite number of cations \((\lesssim 10^3)\), self-averaging of configurations may not be complete, so single-dot spectroscopy can observe the atomic-scale alloy randomness effects. We examine the effect of such atomic-scale randomness on the fine structure-splitting (FSS) of the exciton observed via the polarization anisotropy of its components. We find: (i) The FSS of the monoelecton X\textsuperscript{1}\textsuperscript{+} changes by more than a factor of 7 with \( \sigma \). Thus, finite nanostructure systems provide clear evidence for the effects of atomic-scale randomness on physical properties. (ii) The polarization anisotropy of two X\textsuperscript{1}\textsuperscript{+} transitions is affected both by \( \sigma \) variations and from possible QD base elongation. Thus, the polarization anisotropy cannot be used as a measure of geometrical anisotropy alone, (iii) Polarization directions of different multiexciton emission lines are determined by \( \sigma \).

\textsuperscript{1}Funded by DOE-SC-BES-MSED through NREL Contract DE-AC36-08GO28308

9:24AM H10.00006 Blinking suppression on millisecond-to-minutes time scales in giant nanocrystal quantum dots\textsuperscript{,} ANTON MALKO, University of Texas at Dallas, DAVID BUSSIAN, HAN HTOON, Los Alamos National Laboratory, SID SAMPAT, University of Texas at Dallas, JAVIER VELA, YONGFEN CHEN, JENNIFER HOLLINGSWORTH, VICTOR KLIMOV, Los Alamos National Laboratory — Fluorescence intermittency (blinking) is an intrinsic feature of molecular-like fluorophores, including nanocrystal quantum dots (NQDs). The effect complicates applications of NQDs in areas such as quantum informatics, bio-imaging, and real-time tracking. Previously we developed “giant” NQDs in which a small emitting core is overcoated with a thick shell of a wider-gap material and observed strong blinking suppression on a time scale of 100s ms and longer. In this work, we employ time-tagged correlated single photon counting to detect photoluminescence (PL) traces from individual “giant” CdSe/CdS NQDs with resolution better than 1 ms. We observe a strong dependence of the fluorescence on/off times on shell thickness and almost complete blinking suppression on all measured time scales for NQDs coated with more than \( \sim 10 \) monolayers of CdS. Further systematic analysis of our PL traces reveal a photon statistics that differs significantly from a power-law distribution of on/off times typically observed for “regular” NQDs.

9:36AM H10.00007 Photoluminescence and multiexciton dynamics in semiconductor nanoparticle, MOUNGI BAWENDI, MIT — No abstract available.

10:12AM H10.00008 Scaling of Multiexciton Nonradiative and Radiative Decay Rates with Exciton Number in Semiconductor Nanocrystals\textsuperscript{1}. JOHN A. MCGUIRE, VICTOR I. KLIMOV, Chemistry Division, Los Alamos National Laboratory — Rapid multiexciton decay by nonradiative Auger recombination places strong constraints on potential applications of semiconductor nanocrystals (NCs) in lasing and solar energy conversion exploiting carrier multiplication. Hence, it is important to understand the scaling of the Auger recombination rate with exciton number in NCs. Likewise, understanding the scaling of multiexciton radiative rates with exciton number is important both for potential applications of, e.g., ordered multiphoton emission and for interpreting experimental measurements of time-resolved photoluminescence. We report measurements of the scaling of Auger and recombination rates in CdSe and PbSe NCs and of multiexciton radiative rates in PbSe NCs. The more rapid scaling of Auger rates with exciton number \( N \) in PbSe compared to CdSe can be understood in terms of the different symmetries of \( N \)-excitons with \( N \geq 2 \) due to the different degeneracies of the lowest-energy excitonic states. The scaling of the multiexciton radiative rates in PbSe can be interpreted in terms of a “free-carrier” model.

\textsuperscript{1}This work was supported by the Office of Basic Energy Sciences of DOE, the DOE Center for Integrated Nanotechnologies, and Los Alamos LDRD funds.

10:24AM H10.00009 Carrier Multiplication in PbSe Nanocrystals and Extraneous Processes\textsuperscript{1}, JOHN A. MCGUIRE, JIN JOO, JEFFREY M. PIETRYGA, ISTVAN ROBEL, VICTOR I. KLIMOV, Chemistry Division, Los Alamos National Laboratory — Spatial confinement of electronic wave functions in semiconductor nanocrystals (NCs) can enhance the efficiency of carrier multiplication (CM), a process whereby multiexcitons are generated from single absorbed photons. In the last year, a controversy has emerged due to large discrepancies between values of CM efficiencies reported by different groups using different techniques – transient absorption (TA) and photoluminescence upconversion (uPL). We report studies of CM in solutions of PbSe NCs using measurements of exciton dynamics by both TA and uPL and find excellent agreement between the CM efficiencies extracted by both techniques. Moderate variations in efficiencies are observed for nominally similar samples. More dramatically, measurements of static and stirred solutions can display large differences in dynamics. This indicates that extraneous effects such as NC photoionization can distort the results of CM studies and are a likely contribution to the discrepancies between previously reported CM efficiencies.

\textsuperscript{1}This work was supported by the Office of Basic Energy Sciences of DOE, the DOE Center for Integrated Nanotechnologies, and Los Alamos LDRD funds.

10:36AM H10.00010 Universal size dependence of Auger constants in direct- and indirect-gap semiconductor nanocrystals, ISTVAN ROBEL, Chemistry Division, Los Alamos National Laboratory, RYAN GRESBACK, UWE KORTSHAGEN, Department of Mechanical Engineering, University of Minnesota, RICHARD D. SCHALLER, VICTOR I. KLIMOV, Chemistry Division, Los Alamos National Laboratory — We compare Auger recombination rates in several direct- and indirect-gap semiconductor nanocrystals including Ge, PbSe, InAs, and CdSe. Our size-dependent biexciton lifetime measurements indicate that the most important factor determining recombination rates is nanocrystal size, while details of the materials’ electronic structure such as the width of the energy gap or its direct/indirect nature play only a minor role. We observe that the effective Auger constants for all semiconductor nanocrystals in this study exhibit a universal cubic dependence on particle radius \( R \), \( C_A \sim R^3 \). Moreover, absolute values of nanocrystal Auger constants are comparable across different materials despite a dramatic difference (up to 4-5 orders of magnitude) in \( C_A \) values in the respective bulk solids. Our results can be explained by confinement-induced relaxation of momentum conservation, diminishing the difference between direct- and indirect-gap semiconductors at the nanoscale.
10:48AM H10.00011 Steady-state fluorescence spectroscopy of multiexcitons in single ‘giant’ nanocrystal quantum dots, HAN HTOON, DAVID BUSSIAN, JAVIER VELA-BECERRA, YONGFEN CHEN, JENNIFER HOLLINGSWORTH, VICTOR KLIMOV, Los Alamos National Lab — Due to ultrafast nonradiative Auger recombination, emission of multiexciton states is not pronounced in steady-state spectra of nanocrystal quantum dots (NQDs). Here, we report the first observation of multiexcitonic signatures in steady-state photoluminescence (PL) from single ‘giant’ core/shell NQDs*, in which a CdSe core is overcoated with a thick (>10 monolayers) CdS shell. At low temperature, we observe the emergence of multiple high-energy PL peaks with increasing pump power. Analysis of intensity scaling of these PL peaks with pump power allows us to assign them to bi-, tri- and higher order multiexcitons. Lifetimes of these multiexciton states obtained by single-dot time- and wavelength-resolved PL further corroborate this assignment. These results suggest that in ‘giant’ NQDs Auger recombination is greatly suppressed compared to regular NQDs, which likely stems from their large effective volume and decreased spatial overlap between electrons (occupy entire NQD volume) and holes (localized in CdSe core).* Y.F. Chen et al. J. Am. Chem. Soc. 130, 5026 (2008)

1This work was supported by the DOE Center for Integrated Nanotechnologies (CINT), and Los Alamos LDRD funds.

Tuesday, March 17, 2009 8:00AM - 11:00AM
Session H11 DMP: Focus Session: Transport Properties of Nanostructures II: Molecular Junctions

8:00AM H11.00001 Conductance of Conjugated Organic Compounds in Controlled Environments1, CHRISTIAN SCHONENBERGER, Department of Physics, Univ. of Basel — We use the mechanical and the electromigration break junction technique, as well as nanoparticle arrays, to measure the electrical conductance of a range of conjugated organic molecules with different end functionalities at room temperature in a liquid cell. We first report on a comparison between oligo(phenylene vinylene) (OPV) oligo(phenylene ethynylene) (OPE). We find that OPV conducts slightly better than OPE. Solubilizing side groups do not prevent the molecules from being anchored within a break junction. With the aim to realize a functional switch, we show preliminary electrical conductance studies of a newly synthesized cruciform molecule. Using the nanoparticle platform we further demonstrate light and electrochemical-induced conductance switching of photochromic and redox molecules. We further discuss OPV and OPE molecules with different end groups, including asymmetric ones. To our surprise, molecules having an anchor group only on one side also gave rise to a pronounced mo-lecular signal. We attribute this effect to the interaction between neighboring molecules in the junction likely induced by π-π stacking. This remarkable property highlights the importance of intermolecular interaction in molecular junctions, an often overlooked aspect. If time permits, a recent study on low-frequency fluctuations in molecular junctions will be mentioned as well. Collaborators are (alphabetical order): J. Agustsson, J. Brunner, M. Calame, T. Gonzalez, S. Grunder, V. Horhoiu, R. Huber, J. Liao, M. Mayor, M. Mangold, S. Oberholzer, M. Steinacher, S. Wu, Z.M. Wu, (all at the Swiss Nanoscience Institute at the Univ. of Basel) and M. R. Bryce (Durham University, UK):

1Support by Swiss NSF, ESF, EU-FP7 FUNMOL and FUNMOLS is gratefully acknowledge

8:36AM H11.00002 Externally controlled spin state switching in metal-organic complexes, ALEXEI BAGRETS, VELIMIR MEDED, MARIO RUBEN, FERDINAND EVERS, Institute of Nano Technology, Research Center Karlsruhe, Germany — Recent transport experiments have demonstrated that a manipulation of the charge of individual molecules is feasible using electromigrated metal junctions [1] or electrochemical gates in conjunction with the STM [2]. Using elaborated density functional theory calculations, we will discuss a possibility to induce – by means of charging or applied stress – a switching between low and high spin states in certain metal-organic systems, Fe(bpp)$_2$[2]+ (bpp: bispyrazolyl pyridine) and Mn(tpy)$_2$[2]+ (tpy: terpyridine). Based upon a recent success of the single molecular conduction experiment through Ru(II) complex [3], we anticipate the transport properties of Fe(II) and Mn(II) complexes to be gate controlled via exploiting their spin degree of freedom.


8:48AM H11.00003 ABSTRACT WITHDRAWN —

9:00AM H11.00004 Quantum-Interference-Controlled Molecular Electronics, SAN-HUANG KE, WEITAO YANG, H. U. BARANGER, Duke University — Quantum interference in coherent transport through single molecular rings may provide a mechanism to control the current in molecular electronics. We investigate its applicability, using a single-particle Green function method combined with ab initio electronic structure calculations. We find that the quantum interference effect (QIE) is strongly dependent on the interaction between molecular π-states and contact σ-states. It is masked by σ tunneling in small molecular rings with Au leads, such as benzene, due to strong π – σ hybridization, while it is preserved in large rings, such as [18]annulene, which then could be used to realize quantum interference effect transistors. [Nano Letters 8, 3257 (2008)]

9:12AM H11.00005 Simultaneous electronic transport and Raman spectroscopy in single-molecule devices, DOUGLAS NATIELSON, Rice University, Dept. of Physics and Astronomy — Over the last decade several techniques have been developed to examine electronic transport through individual small molecules. These include scanned probe methods, mechanical break junctions, and electromigrated junctions. One recurring challenge is the need to confirm that current flow is, indeed, through the molecule of interest rather than a contaminant. We recently discovered (D. R. Ward et al., Nano Lett. 7, 1396 (2007)) that the same electromigrated Au source and drain electrodes used for transport are tremendously effective optical antennas in the near infrared. Surface plasmon modes localized to the nm-scale interelectrode gap lead to large enhancements of the local electric field relative to that from incident radiation. The result is that these nanoscale gaps are tremendous “hot spots” for surface-enhanced Raman scattering (SERS). We perform simultaneous measurements of electronic transport and SERS in junctions incorporating molecules of interest, and find in 10-15% of devices that the conductance and SERS emission are strongly correlated in time (D. R. Ward et al., Nano Lett. 8, 919 (2008)). Since the conductance mechanism is tunneling and therefore dominated by a volume comparable to that of a single molecule, this strongly implies that the SERS emission comes from that same molecule. The distinctive SERS spectra allow us to confirm that conduction in these devices is through the molecule of interest. Furthermore, these devices open up many opportunities, including studies of electron-vibrational couplings and dissipation at the single-molecule level.

2This work was done in collaboration with D. R. Ward, N. J. Halas, P. Nordlander, and J. M. Tour. Financial support includes Robert A. Welch Foundation grant C-1636, NSF DMR-0347253, and the David and Lucille Packard Foundation.
Films 308 appears whenever a conductance channel is opened.

with the peak index in the conductance histogram. The present study shows that the [110] nanowire behave as ballistic conductors, and a conductance peak either an atomic sheet or a hexagonal prism. The number of conductance channels calculated for each atomic structure by first principles theory, coincided well =2e microscrope images. The conductance histogram exhibits a series of peaks whose conductance values increased nearly in steps of the conductance quantum, G0 elongated along the [110] direction (gold [110] nanowire) was measured during many breaking procedures, while simultaneously acquiring transmission electron microscope images. The conductance histogram lineshapes show strong correlation between measured conductance step length and molecular backbone length, with phosphine link groups showing longer steps than amine link groups. We model adiabatic junction evolution by discrete steps, with structure determined by energy minimization in a DFT approach and the low bias junction conductance at each step computed using a Green’s function approach. We identify different mechanisms whereby the attachment point to the electrode can shift while maintaining similar conductance, explaining why conductance steps can extend over distances of several angstroms. Phosphine and amine link groups sustain different maximum forces, accounting for key differences in junction evolution.

Kondo effect in the electronic transport of magnetic atomic-size contacts

M. REYES CALVO, JOAQUIN FERNANDEZ-ROSIER, JUAN JOSE PALACIOS, Dept. Fisica Aplicada. Universidad de Alicante, DAVID JACOB, Dept. Physics and Astronomy. Rutgers University, DOUGLAS NATELSON, Dept. Physics and Astronomy. Rice University., CARLOS UNTIEDT, Dept. Fisica Aplicada. Universidad de Alicante — Low coordination alters dramatically the magnetic properties of materials at the nanoscale. Our results indicate that, in the case of atomic contacts of certain materials, a localized magnetic moment appears at the contact and is screened at low temperatures by means of the Kondo effect. We observe characteristic Fano-Kondo lineshapes in the spectroscopy of atomic contacts of typical ferromagnetic materials (Fe, Co and Ni). The parameters obtained from the fitting of these curves to the Fano equation show statistical distributions that agree with the Kondo theory. The Kondo origin of the measured resonances is confirmed by their temperature dependence and supported by our theoretical calculations. These results are surprising since ferromagnetism and Kondo effect are expected to compete. We have also observed a similar spectroscopy in atomic contacts of palladium and platinum monoatomic chains. In this case, the Kondo resonances would be the signature of an emergent magnetism that is ultimately screened. Partially founded by Spanish MEC (grant nr. MAT2007-65487 and CONSOLIDER CSD2007-0010) and EU (project nr. 211284).

Magnetic phenomena, ferro and antiferro Kondo, and transport in transition metal break junction nanocontacts


Spectra of discrete electrons-in-a-box energy levels in chemically-formed Au and Pt nanoparticles.

SU-FEI SHI, F. KUEMMETH, K.I. BOLOTIN, W. LI, D.C. RALPH, Cornell University — We report tunneling spectroscopy measurements of the discrete electron spectra of individual metal nanoparticles formed by chemical synthesis, that they are well-defined in their composition, size, and shape. The spectra of 5-15 nm diameter gold particles exhibit as many as 40 resolvable electronic excited states for a fixed value of gate voltage. We find excellent agreement between the measured level statistics and random matrix predictions for the regime of strong spin-orbit coupling and ballistic transport. As a function of changing gate voltage, the energy-level spectra in the Au particles are not scrambled by the addition of electrons, indicating that in these particles the variation in the strength of electron-electron interactions between states is negligible. We have also succeeded in fabricating single-electron transistors from individual Pt nanoparticles and hope to present measurements of their discrete spectra. Unlike Au, has a sufficiently strong exchange interaction that it is expected to exhibit non-zero values of the ground state spin in the form of “mesoscopic magnetism”.

Ballistic transport in gold [110] nanowire

YOSHIHIKO KURUI, YOSHIFUMI OISHIMA, Tokyo Institute of Technology, MASAKUNI OKAMOTO, Hitachi Ltd, KUNIO TAKAYANAGI, Tokyo Institute of Technology — Conductance of gold nanowire elongated along the [110] direction (gold [110] nanowire) was measured during many breaking procedures, while simultaneously acquiring transmission electron microscope images. The conductance histogram exhibits a series of peaks whose conductance values increased nearly in steps of the conductance quantum, G0 =2e2/h. However thick nanowires above 10G0 showed dequantization, where the increment was only 0.9G0. The structure for each peak was determined to be either an atomic sheet or a hexagonal prism. The number of conductance channels calculated for each atomic structure by first principles theory, coincided well with the peak index in the conductance histogram. The present study shows that the [110] nanowire behave as ballistic conductors, and a conductance peak appears whenever a conductance channel is opened.

Tuesday, March 17, 2009 8:00AM - 11:00AM –
Session H12 DMP DCMP: Focus Session: Directed Organization of Molecular Semiconductor Films 308
8:00AM H12.00001 Structural evolution of the self-assembled layers of functionalized fullerenes on metal surfaces , BOGDAN DIACONESCU, Department of Physics, University of New Hampshire, MIKAEL JAZDZYK, GLEN MILLER, Department of Chemistry, University of New Hampshire, KARSTEN POHL, Department of Physics, University of New Hampshire — Self-assembled organic thin films have a great number of practical applications, ranging from sensors and biological interfaces to medical implants to organic electronics and photovoltaics. Self-assembled monolayers (SAMs) form as a result of a delicate balance between competing molecule-substrate and intermolecular interactions. To control such self-assembly processes, it is mandatory to understand how this balance reflects onto the SAM’s final structure. Here, we present a STM study of the self-assembly of C60 functionalized with alkane chains of various lengths (F-C60) on Ag(111). We find that F-C60 molecules lay down on the Ag surface and form a zigzag like pattern with an oblique unit cell of size dependent on the alkyl chain length and two molecules per basis. The C60s are placed at a larger than van der Waals distance. The symmetry of the F-C60 SAM is dictated by the alkane-surface interaction while the size of the unit cell is a consequence of the intermolecular interactions. These results show that C60s can be assembled in 2D and non-compact molecular arrays with a surface density controllable via appropriate chemical functionalization. Funded by the NSF Center for High-rate Nanomanufacturing (NSF NSEC-425826).

8:12AM H12.00002 Controlled Chemical Morphology in TiO Pc - C60 Films , YINYING WEI, Department of Chemistry and Biochemistry, University of Maryland , STEVE ROBEY, National Institute of Standards and Technology, JANICE REUTT-ROBEY, Department of Chemistry and Biochemistry, University of Maryland — A key strategy for the improvement of organic electronic devices involves the optimization of chemical morphology for efficient charge separation. Fundamental studies of chemical morphology - electronic property relations, particularly along crucial domain boundaries, are needed to realize these goals. We present STM/STS studies of TiO Pc: C60 films, prepared by vapor deposition on Ag (111). We show how growth conditions can be adjusted to harness anisotropic TiO Pc - TiO Pc interactions, leading to three dramatically distinct film structures: nanophase segregated TiO Pc and C60 domains, a co-crystalline TiO Pc(C4H9)2-C60(111) honeycomb network, and a quasi-periodic array of triangular TiO Pc domains and C60 nanoclusters. Electronic transport gaps measured by STS (Z(V)) prove to be sensitive to the phase, varying by up to about 0.5 eV along domain boundaries. We propose structural models for each hetero interface and discuss the physical origin of the observed transport characteristics.

8:24AM H12.00003 Monte Carlo Study of the Honeycomb Structure of Anthraquinone Molecules on Cu(111) , KWANGMOO KIM, T. L. EINSTEIN, University of Maryland, College Park, LUDWIG BARTELS, University of California, Riverside — Using Monte Carlo calculations of the two-dimensional (2D) lattice gas model, we demonstrate a mechanism for the spontaneous formation of honeycomb structure of anthraquinone (AQ) molecules on a Cu(111) plane. Unlike the suggestion of long-range substrate-mediated repulsion, long-range attractions play important roles in our calculations. However, the interplay between attractions and repulsions is still integral to the spontaneous formation of AQ’s honeycomb structure. We also compare the critical local coverage rate of AQ’s where the honeycomb structure starts to form. Furthermore, we study the diffusion of CO molecules inside AQ honeycombs on the Cu(111) plane. The surface phase transitions of CO molecules between solid, liquid, and gas 2D phases are studied via the specific heat singularity in short-range correlation functions. Supported primarily by NSF Grants CHE07-50334 with a secondary support from MRSEC Grant DMR05-20471.

8:36AM H12.00004 Patterned molecular nanostructures , KLAUS KERN, Max Planck Institute for Solid State Research and EPFL (Switzerland) — Surfaces and interfaces not only determine to a large extent the properties of small-scale materials due to their high surface-to-volume ratio, they are also an ideal platform for the design, fabrication and device integration of nanostructures. Both, top-down and bottom-up methods have been developed for the handling of matter at the molecular and atomic scale. In the present talk I will demonstrate how the remarkable progress in controlling atomic and molecular interactions at surfaces has provided the unique ability to engineer supramolecular architectures of well-defined shape, size, composition and functionality. Using noncovalent interactions as hydrogen bonding, ionic bonding and metal-ligand interactions, molecular building blocks can be rationally combined into desired functional architectures. The potential functionalities comprise molecular magnetism, novel heterogeneous catalysis, selective host-guest interactions and new concepts of nanoscale mechanics.

9:12AM H12.00005 Reactions on surfaces for the creation of stable templates , M. MATENA, M. WAHL, M. STOEHR, Universität Basel, Switzerland, T. A. JUNG, Paul-Scherrer-Institute, Switzerland, T. L. LEE, J. ZEGENHAGEN, ESRF Grenoble, France, T. RIEHM, L. H. GADE, University of Heidelberg, Germany — Molecular assemblies on surfaces can be used as templates that allow the study of host-guest interactions and thus provide a starting point for the generation of complex hierarchic structures. An important prerequisite besides the regularity of such structures is their stability. We reported the formation of a molecular network generated by thermal dehydrogenation of a perylene derivative (DPDI) on a substrate surface before and after the thermal activation. The formation of the network involves a lowering of the height difference utilizing this network for the incorporation of guest molecules. NIXSW (normal incidence x-ray standing wave) experiments were carried out to determine the appropriate chemical functionalization. Funded by the NSF Center for High-rate Nanomanufacturing (NSF NSEC-425826).

9:24AM H12.00006 Meandering C60 Chains on Organic Film Substrates , WEI JIN, University of Maryland, DANIEL DOUGHERTY, National Institute of Standards and Technology (currently at North Carolina State University), QIANG LIU, WILLIAM CULLEN, JOHN WEEKS, University of Maryland, STEVEN ROBEY, National Institute of Standards and Technology, JANICE REUTT-ROBEY, University of Maryland — Meandering chains of C60 molecules are observed following vapor deposition of C60 on a variety of organic molecular films including pentacene and zinc phthalocyanine, as well as previously reported a-selenophene. Such filamentous structures are in complete contrast to C60’s typical close-packed growth habit, but are reminiscent of dipole fluids. We present STM images and a statistical analysis of chain structures observed for 0.2 - 0.9 mL C60 overlayers (a = 13.6 Å, b = 14.5 Å, α = 89°) on Ag (111). Large islands of meandering C60 islands indicate >50 nm C60 diffusion lengths on this ZnPc film. The C60 island length, ~20 nm, depends weakly on coverage, reflecting the ~constant C60 density within these islands, and exhibits multiple branches. Chain structures are compared to the molecular dynamics predictions of a 2-d dipole fluid with the C60 - C60 interaction described by the Girifalco Potential (1 eV attraction) with additional dipole terms. A vertical moment of ~0.8 D simulates filament formation. The structure of the ZnPc support, not included in this simulation, appears to be a secondary consideration in these chain structures. Supported by the Dept. of Commerce through the NIST Center of Nanomanufacturing and Metrology and the NSF-funded MRSEC via DMR-05-20471.
9:36AM H12.00007 Molecular dynamics study of polarized C60 on an organic surface1. QIAN LIU, WEI JIN, JOHN D. WEEKS, JANICE REUTT-ROBEY — The experimental results of vapor deposition of C60 on a variety of organic molecular films has showed unusual meandering chain structures. Here we use the Langevin molecular dynamics method to mimic the system. In the simulation, we considered interactions including the intermolecular Girifalco potential, dipole-dipole interactions, octupole interactions suggested by W. Losert2 and substrate potentials. Choosing different parameters can give us different C60 patterns: the close-packed C60 islands, isolated C60 molecules and meandering chain islands.

1This work is supported by UMD MRSEC under Grant DMR 05-20471. 2J.Stambaugh, Z.Smith, E.Ott and W.Losert, Phys.Rev.E 70, 031304

9:48AM H12.00008 Harnessing Surface Dislocation Networks for Molecular Self-Assembly1. KARSTEN POHL. University of New Hampshire — The controlled fabrication of functional wafer-based nano-arrays is one of the ultimate quests in current nanotechnologies. Well-ordered misfit dislocation networks of ultrathin metal films are viable candidates for the growth of two-dimensional ordered cluster arrays in the nanometer regime. Such bottom-up processes can be very complex, involving collective effects from a large number of atoms. Unraveling the fundamental forces that drive these self-assembly processes requires detailed experimental information at the atomic level of large ensembles of hundreds to thousands of atoms. The combination of variable temperature measurements from our home-built STM correlated with 2D Frenkel-Kontorova models based on first-principle interaction parameters is used to explain how uniform arrays can form with the strain in the thin film as the driving force responsible for the surface self-assembly process. This process is generally applicable to assemble many molecular species thus opening avenues towards complex self-assembled structures based on a lock-and-key type approach. Moreover, when increasing the molecular coverage and/or decreasing the strain in the thin film the intermolecular interactions will eventually dominate the elastic effects and dictate the self-assembly process via molecular structure and functionality. We will show that controlling this delicate balance leads to a richness of structures, ranging from disordered arrays of molecular clusters to patterned self-assembled monolayers (SAMs) of functionalized fullerenes and methanethiol.

1This work is supported in parts by the NSF-DMR and the Center for High-rate Nanomanufacturing (NSF-NSEC-425826).
8:12AM H13.00002 Iterative Diagonalization of Inhomogeneous Heisenberg Models1, VALTER LIBERO, FABIANO SOUZA, Universidade de Sao Paulo — The antiferromagnetic Heisenberg model is one of the most important in describing quantum spins coupled by exchange interactions. Difficulties arise especially in presence of broken symmetry, due for instance to impurities or defects. In these cases, even well-established numerical methods like Lanczos or Monte Carlo, encounter limitations. We propose a numerical method which works even in the absence of translational invariance. We diagonalize the Heisenberg model exploiting the conservation of both the z-component of the total spin and the square of the total spin, a much more complicated procedure but that renders an additional block diagonalization. In essence, the N-site Hamiltonian is built using basis-vectors generated from the direct product of the eigenvectors of the (N-1)-site Hamiltonian and the states of the added N-th spin. The procedure is also applied for the two-leg ladder, an experimental relevant system. Results are shown for ground-state energy and temperature dependent specific heat for chains with local spin impurities or with random distributions of spins 1/2, 1 or 3/2.

8:24AM H13.00003 Entanglement perturbation theory for the excitation spectrum in one dimension, SUNG CHUNG, Western Michigan University — A novel many-body method, entanglement perturbation theory, is developed for the excitation spectra in one dimension. Applied to the antiferromagnetic Heisenberg chains with spin one-half and 1, converging and hence exact results are obtained, including known Bethe Ansatz result for spin one-half and DMRG results for spin 1. We have found that the magnons are spread over about 4 lattice sites. An essential ingredient in this theory is the exact, un-renormalized ground state of arbitrary system sizes, which are also calculated by EPT in a simple, general and exact manner.

8:36AM H13.00004 A Brief Introduction to the Truncated Eigenfermion Decomposition1, JONATHAN E. MOUSSA, JAMES R. CHELIKOWSKY, UT Austin — We present a computational formalism for the approximate unitary transformation of a many-body fermion Hamiltonian with two-body interactions. This work is a further development of the numerical canonical transformation approach of S. R. White [J. Chem. Phys. 117, 7472 (2002)]. The Hamiltonian can be diagonalized in a basis of eigenfermion operators, in which case the eigenstates are all single Slater determinants of eigenfermions. The transformation of two-body interactions generates higher-order interactions that can be approximated by effective two-body interactions using a novel generalization of normal ordering. The error in representing a target eigenstate is minimized by performing the generalized normal ordering with respect to that eigenstate. Numerical results are presented for several test cases, including Hubbard model clusters.

8:48AM H13.00005 The Density Matrix Renormalization Group Algorithm for Strongly Correlated Systems: A Generic Implementation1, GONZALO ALVAREZ, Oak Ridge National Laboratory — I will present DMRG++, a fully functional generic Density-Matrix Renormalization Group (DMRG) code with sample cases for the Hubbard and Heisenberg model, and for one-dimensional chains and n-leg ladders. My talk will include an overview of the core C++ classes, effective symmetry blocking and parallelization found in DMRG++. I will also explain how to add new strongly correlated electron (SCE) models and geometries with minimal code changes. Even if you are not very familiar with the DMRG or C++, you will be able to understand the main motivations and advantages of generic programming applied to SCE systems.

3Supported by the Center for Nanophase Materials Sciences, sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. Department of Energy, under contract with UT-Battelle.

9:00AM H13.00006 A Renormalization Group for Treating 2D Coupled Arrays of Continuum 1D Systems, ROBERT KONIK, YURY ADAMOV, Brookhaven National Laboratory — We study the spectrum of two dimensional coupled arrays of continuum one-dimensional systems by wedging a density matrix renormalization group (DMRG) procedure to a renormalization group improved truncated spectrum approach. To illustrate the methodology we study the spectrum of large arrays of coupled quantum Ising chains. We demonstrate explicitly that the method can treat the various regimes of chains, in particular the three dimensional Ising ordering transition the chains undergo as a function of interchain coupling. We argue that the methodology’s success is based on finite size corrections being exponentially small which in turn allows the block DMRG entanglement entropy to be kept to a minimum.

9:12AM H13.00007 Low-temperature density matrix renormalization group using regulated polynomial expansion, SHIGETOSHI SOTA, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University — We propose a new scheme of density matrix renormalization group (DMRG) for low dimensional strongly correlated electron systems at finite temperatures, which is a straightforward extension of the target-state procedure at zero temperature. In order to investigate thermodynamical properties, we employ the target state that is weighted by a Boltzmann factor [1]. Making use of a regulated polynomial expansion [2] and random sampling, we can calculate static and dynamical quantities at finite temperatures. In order to obtain good convergence in high temperature region, we need a large truncation number of the density matrix, while a necessary truncation number is small at low temperatures. The proposed method is, therefore, suitable for lower temperature region. As a demonstration of the method, we show the specific heat and dynamical current-current correlation function of the 1D Hubbard model at half filling. The DMRG results reproduce the exact digitalization results at low temperatures. [1] S. Sota and T. Tohyama, Phys. Rev. B 78, 113101 (2008). [2] S. Sota and M. Itoh, J. Phys. Soc. Jpn. 76, 054004 (2007).

9:24AM H13.00008 Screened Coulomb Interactions of Localized Electrons from First-Principles, BI-CHING SHIH, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York — We present a recently developed, maximally localized Wannier function approach for calculating the screened Coulomb(U) and exchange (J) interactions of localized electrons in solids. The localized orbitals are constructed using the maximally localized Wannier function approach. The dielectric screening is calculated from first-principles within the random phase approximation. Results for several systems containing strongly localized d electrons will be presented.

9:36AM H13.00009 Refinement of a Lanczos-based variational procedure to solve the Holstein model, ZHOU LI, University of Alberta, DEVIN BAILLIE, University of Alberta, CINDY BLOIS, University of Toronto, FRANK MARSIGLIO, University of Alberta — We propose a slight refinement to the Trugman variational procedure to more efficiently solve the Holstein model with Lanczos methods. The modified Lanczos method converges much more quickly compared with the usual one in the intermediate- and strong- coupling regimes. To get a 6-digit accuracy of ground state energy at intermediate-strong coupling in the adiabatic region (small phonon frequency), only about 5000 basis states are need to be included. We also construct a variational ground state based on the numerical results.
of like-charge attraction: the charge-dependent term in the interaction is purely repulsive, while the attraction is independent of particle charge. We report a decomposition of like-charge interactions into charge-dependent and -independent terms, leading to a striking insight into the long-standing paradox of lipid composition allowing the first self-assembled microparticle superstructures remains slow, however, and fundamental mysteries such as the attractions observed between like-charged particles and scientific importance of colloidal materials has spurred a large body of research into the functionalization of micron-scale particles. Progress towards self-assembled microparticle superstructures remains slow, however, and fundamental mysteries such as the attractions observed between like-charged particles and the large cluster is calculated using the Schwinger-Dyson equation. The method is applied to the 2D Hubbard model with cluster sizes $N_c^{(2)} \geq N_c^{(1)}$ and the results are compared with those calculated using QMC by increasing the size of the small cluster $N_c^{(1)}$ up to $N_c^{(2)}$. 1Supported by DOE SciDAC Grant #DE-FC02-06ER25792.

10:12AM H13.00012 Nonlinear conductance oscillation in strong correlation limit of molecular quantum dots near zero bias anomaly1, JONG E. HAN, SUNY at Buffalo — Recent experiments on strong correlation effects in molecular junctions have demonstrated that the interplay of electronic coupling to molecular vibrations and the Coulomb interaction produces intriguing oscillatory structures in the nonlinear conductance near zero bias anomaly at voltages in the energy scale of, presumably, the Kondo temperature. Using the imaginary-time quantum Monte Carlo technique recently developed for strongly correlated nonequilibrium, the nonlinear conductance of the Anderson-Holstein model at finite bias has been calculated. We discuss the mapping between the charge- and spin-Kondo limits and their distinctly different transport physics under finite chemical potential bias. We show that the conductance oscillation emerges at finite bias in the vicinity of the Kondo temperature due to strong electron-vibration coupling. The origin of the oscillation is from the bias-induced strong electron density modes as opposed to direct phonon excitations.

1Supported by NSF DMR-0426826.

10:24AM H13.00013 Role of phonons and of finite temperature on the spectral function of a single hole in a 2D quantum antiferromagnet, SATYAKI KAR, Department of Physics, FSU & MARTECH, EFSTRATIOS MANOUSAKIS, Department of Physics, FSU & MARTECH, Department of Physics, University of Athens, Greece — We study thermal broadening of the hole spectral function of the two-dimensional $t-J$ and $t-t'$ - $J$ model within the non-crossing approximation (NCA) with and without the contribution of optical phonons. We have also studied the range of validity of the NCA by including the role of vertex corrections. The broadening of the quasiparticle peak as well as the transfer of spectral weight as a function of momentum to higher energy string excitations is found to be in reasonably good agreement with experimental angle resolved photo-emission spectroscopy (ARPES) results using a rather large electron-phonon coupling.

10:36AM H13.00014 Inelastic Scattering from Local Vibrational Modes, BALAZS DORA, MIKLOS GULACSI, Max Planck Institute for the Physics of Complex Systems — We study a nonuniversal contribution to the dephasing rate of conduction electrons due to local vibrational modes. Bosonization allows us to evaluate the full T-matrix. The inelastic scattering rate is strongly influenced by multi phonon excitations, exhibiting oscillatory behaviour. For higher frequencies, it saturates to a finite, coupling dependent value. In the strong coupling limit, the phonon is almost completely softened, and the inelastic cross section reaches its maximal value. This represents a magnetic field insensitive contribution to the dephasing time in mesoscopic systems, in addition to magnetic impurities.

Tuesday, March 17, 2009 8:00AM - 10:36AM – Session H14 DFD: Colloids III: Formation and Control 315

8:00AM H14.00001 Connecting structure and rheology in sheared colloidal suspensions, JONATHAN MCCOY, ITAI COHEN, Cornell University — We investigate the shear properties of colloidal suspensions confined between parallel plates. When the distance between the plates is very small, i.e. approaching the size of the colloidal particles, a number of dramatic phase behaviors are observed under shear, including buckling, banding, jamming, and crystallization. This strongly confined regime is difficult to access using standard rheological techniques. Our experiment explores connections between microstructural behaviors and macroscopic flow by combining confocal microscopy and force measurement techniques in a custom-built thin-film shear cell. Here, we will focus on the interplay between confinement, slip, and order.

8:12AM H14.00002 Modulation of attractive colloidal interactions by lipid and protein membrane functionalization, YUPENG KONG, RAGHUVEER PARTHASARATHY, Univ. of Oregon, Dept. of Physics — The broad technological and scientific importance of colloidal materials has spurred a large body of research into the functionalization of micron-scale particles. Progress towards self-assembled microparticle superstructures remains slow, however, and fundamental mysteries such as the attractions observed between like-charged particles near a confining wall remain unresolved. These difficulties arise in large part due to the lack of experimental systems with tunable, attractive interparticle interactions. Biomembranes are appealing candidates for colloidal functionalization, enabling access to electrostatic and chemical properties that influence inter-particle relations. We describe here the first measurements of the pair interaction energy for membrane-functionalized colloids, using a newly developed optical line trapping technique. Two classes of particles, derivatized with lipid-only and lipid-plus-protein membranes, each show attractive interactions. The two particle types exhibit different relations between the depth and spatial range of the interactions, however. Control of lipid composition allows the first reported decomposition of like-charge interactions into charge-dependent and -independent terms, leading to a striking insight into the long-standing paradox of like-charge attraction: the charge-dependent term in the interaction is purely repulsive, while the attraction is independent of particle charge.
8:24AM H14.00003 Self-protected interactions in DNA-functionalized colloids: Nano Contact Glue. MIRIAM LEUNISSEN, Center for Soft Matter Research, New York University, REMI DREYFUS, ROUJIE SHAH, New York University, ALEXEI TKACHENKO, University of Michigan, NADRIAN SEE-MAN, DAVID PINE, PAUL CHAIKIN — The ability of single-stranded DNA to form a variety of sequence-dependent secondary structures, such as hairpins, is frequently used in DNA nanotechnology, but has so far not been explored for the directed assembly of (nano)colloidal structures. We will show how mono- and bimolecular hybridization events in the DNA coatings of individual micrometer-sized beads can give rise to unusual, quench-rate dependent aggregation behavior, and how it can give additional control over the colloidal self-assembly process. For example, it provides us with ‘self-protected’ interactions that are activated by temperature or prolonged proximity and that facilitate the formation of finite-sized structures. A simple quantitative model describes the underlying competition between intra- and interparticle hybridization events, based on the known thermodynamic parameters of the DNA sticky ends.

8:36AM H14.00004 A simple quantitative model for the reversible association of DNA coated colloids. REMI DREYFUS, MIRIAM LEUNISSEN, ROUJIE SHAH, New York University, ALEXEI TKACHENKO, University of Michigan, NADRIAN SEE-MAN, DAVID PINE, PAUL CHAIKIN — New York University — We investigate the reversible association of micrometer-sized colloids coated with complementary single-stranded DNA ‘sticky ends’ as a function of the temperature and the sticky end coverage. We find that even a qualitative description of the dissociation transition curves requires the inclusion of an entropic cost. We develop a simple general model for this cost in terms of the configurational entropy loss due to binding and confinement of the tethered DNA between neighboring particles. With this easy-to-use model, we demonstrate for different kinds of DNA constructs quantitative control over the dissociation temperature and the sharpness of the dissociation curve, both essential properties for complex self-assembly processes.

8:48AM H14.00005 Observation of condensed phases of quasi-planar core-softened colloids. PRIMOZ ZIHERL, University of Ljubljana & Jozef Stefan Institute, NATAN OSTERMANN, DUSAN BABIC, IGOR POBERAJ, University of Ljubljana; JURE DOBNIKAR, Jozef Stefan Institute — We experimentally study the condensed phases of repelling core-softened spheres in two dimensions. The dipolar pair repulsion between superparamagnetic spheres trapped in a thin cell is induced by a transverse magnetic field and softened by suitably adjusting the cell thickness. We scan a broad density range and we materialize a large part of the theoretically predicted phases in systems of core-softened particles, including expanded and close-packed hexagonal, square, chain-like, stripe/labyrinthine, and honeycomb phase. Further insight into their structure is provided by Monte Carlo simulations.

9:00AM H14.00006 In situ real time measurement of temperature responsive nanoparticles. DENIS PRISTINSKI, THOMAS Q. CHASTEK, VIVEK PRABHU, KALMAN MIGLER, Polymers Division, NIST — In this work, we combine dynamic light scattering (DLS) and diffusing wave spectroscopy (DWS) to evaluate the size of temperature responsive nanoparticles over a broad range of concentrations. A fiber optic probe DLS instrument was previously demonstrated to measure nanoparticle solutions at a relatively high concentration. The incorporation of back-scattering DWS further extends the technique application to highly turbid conditions. The combined setup was designed to have a simplified and compact optical arrangement employing single-mode fiber based components. Data analysis for both methods was carried out using integrated open source cross-platform software. Measurements were conducted to monitor the progress of poly(N-isopropyl acrylamide) nanoparticle syntheses, including a multi-step seeded polymerization, commonly used to prepare core-shell particles. These particles have received a lot of attention due to their potential for use as targeted drug delivery systems. It was found that DLS and DWS were in good quantitative agreement, and able to accurately characterize the samples.

9:12AM H14.00007 Enhanced particle transport in an oscillating sinusoidal optical potential. WEIQIANG MU, Northwestern University, LAN LUAN, Northwestern University, GANG WANG, Indiana University, Purdue University, Fort Wayne, GABRIEL SPALDING, Illinois Wesleyan University, JOHN KETTENOR, Northwestern University, NORTHWESTERN UNIVERSITY COLLABORATION, INDIANA UNIVERSITY, PURDUE UNIVERSITY, FORT WAYNE COLLABORATION, ILLINOIS WESLEYAN UNIVERSITY COLLABORATION — We have studied the delivery of a colloidal particle in the presence of an oscillating, spatially periodic, optical potential. The average particle velocity relative to the fluid velocity in this potential depends greatly on the oscillation amplitude and frequency. The results of both our simulations and experiments show that for some combinations of these parameters, the average particle velocity can be enhanced due to the synchronization of the particle movement with the oscillating potential.

9:24AM H14.00008 Charge inversion in monovalent ionic solutions1, ALEX TRAVESSET2, Iowa State University and Ames Lab, ALBERTO MARTIN-MOLINA, Universidad de Granada, CARLES CALERO, JORDI FARAUDO, Institut de Ciencia de Materials de Barcelona, MANUEL QUESADA-PEREZ, Universidad de Jaen, ROQUE HIDALGO-ALVAREZ, Universidad de Granada — We present measurements of the mobility of core-softened spheres in the presence of monovalent salt added to the mobility of nearly-spherical (TACl) core-softened colloids with increasing salt concentration that flips sign (charge inversion) at mM salt concentrations. A modified version of the O’Brien and White theory taking into account the hydrophobic nature of the phenyl groups describes the experimental data without fitting parameters. Saturation effects in the mobility as well as possible generalizations are also discussed.

9:36AM H14.00009 Position Control of Particles embedded in Microbeads and Fibers Produced by Electrohydrodynamics.1, UNYONG JEONG, EUN MIN JO, SUNGWON LEE, KYU TAE KIM, Department of Material Science and Engineering, Yonsei University, Seoul, Korea — Electrohydrodynamics is a good approach to produce uniform-sized colloids and fibers in a continuous process. The dimension can be controlled from tens of nanometers to a few micrometers. The structure of the colloids and nanofibers from electrohydrodynamics has been diversified according to the uses. Especially, core-shell structure and hybridization with functional nanomaterials are fascinating due to their possible uses in drug-delivery systems, multifunctional scaffolds, organic/inorganic hybrids with new functions, and highly sensitive gas- or bio-sensors. This talk will present the structural variations by tuning the position of small particles in the colloids and fibers produced from electrohydrodynamics and demonstrate their possible applications.

This work was supported in part by KOSEF grant (No. ROI-2007-001-11281-0) funded by MOST and Seoul R&BD Program(10816).

9:48AM H14.00010 Using colloids to model atomic thin film growth. RAJESH GANAPATHY, MARK BUCKLEY, ITAI COHEN, Cornell University — We epitaxially grow colloidal thin films by sedimenting micron sized colloidal particles on a microfabricated substrate. The attractive interaction between the colloids, induced by a depletant polymer, leads to the nucleation of islands that grow and coalesce with one another. We use confocal microscopy and particle tracking to study the dynamics of the colloidal particles as they diffuse, aggregate and rearrange configurations during deposition. The saturation island density is estimated as a function of the deposition rate and depletant concentration. We find that our results are in excellent agreement with those obtained from atomic deposition experiments suggesting that our system can be used to model various phenomena that occur in atomic thin film growth. Furthermore, we quantify the Ehrlich-Schwoebel step edge barrier by using holographic optical tweezers to create artificial islands and study the dynamics of colloidal monomers placed on the edge of these islands. Owing to the short-range of the attractive interaction in our system, the origin of the step edge barrier in colloids is strikingly different from atoms.
10:00AM H14.00011 Stochastic Rotational Dynamics Simulations of Nanocolloid Suspensions

JEREMY B. LECHMAN, MATT K. PETERSEN, STEVEN J. PLIMPTON, P. RANDALL SCHUNK, GARY S. GREST, Sandia National Laboratories, PIETER IN'T VELD, Polymer Research, BASF — The use of nanoparticle suspensions to potentially tailor the functionality of composite devices has broad applicability, but is limited in practice, in part, due to poor understanding of the phenomena at that scale. In order to address this we have implemented a mesoscale fluid technique called Stochastic Rotation Dynamics (SRD). Here, we discuss the use of this method to investigate the behavior of hard sphere like nanocolloids. In particular we will present a direct, “one-to-one” comparison of an SRD fluid with an explicit Lennard Jones solvent. For small colloids in this low viscosity fluid no “telescoping of timescales” is required for efficiency, which allows us to consider the accuracy of the base numerical scheme without complicating approximations. We present the diffusion and reduced viscosity as a function of volume fraction of colloids and compare to well known results. The efficiency of an SRD simulation relative to an explicit atom simulation is also discussed.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.

10:12AM H14.00012 Light-induced structure transformation of colloidal nanocrystals by using generalized Ewald-Kornfeld formulation

M.J. ZHENg, K.L. CHAN, K.W. YU, The Chinese University of Hong Kong — When metallic nanoparticles are brought close together and they are illuminated by laser light, there will be strongly enhanced forces between these particles [1]. If these particles are suspended in a liquid, the force can promote aggregation. As a result, the cluster size can exceed the wavelength of light and retardation effect must be considered. For this sake, we derived a generalized Ewald-Kornfeld summation [2] which is valid for fully retarded electromagnetic interaction. More importantly, we have extended the formula for a many-point basis in a unit cell. We used the formula to study the colloidal nanocrystal formation and transition driven by surface plasmon resonance enhanced forces. Our results are of fundamental importance to the relevant topics in soft matter physics and can be widely applied in the research of light-induced manipulation.


1Work supported by the General Research Fund of the Hong Kong SAR Government

10:24AM H14.00013 Universal Nanocolloid Deposition Patterns: Harmonics of a Taylor Cone and Separation of DNA-Hybridized Nanocolloids

XINGUANG CHENG, HSUEH-CHIA CHANG, University of Notre Dame — With judiciously placed far-field electrodes, harmonics of the Laplace equation are selected near a conducting Taylor cone with discrete polar angles for the field maxima. Charged nanocolloids ejected along the discrete electric field lines of these mode maxima are observed to deposit a universal spectrum of rings on an intersecting plane, with particles of different size occupying different spectral lines due to different residue charge. After an affine transformation, nanocolloids ejected into a microslit and deposited onto one substrate exhibit the same universal line spectra. The size-selective deposition pattern is used to quantify DNA hybridization yield onto oligo-functionalized nanocolloids.

3This work was supported by the DTRA (HDTRA1-08-C-0016).

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H15 GMAG: Low Dimensional Magnetism (including molecules and surfaces) 316

8:00AM H15.00001 Reversible switching of charge states of single TCNE molecules on Cu(111)

TAEOYOUNG CHOI, JAY GUPTA, Ohio state university — The interplay of electronic structure and magnetic properties is of interest in various organic materials. TCNE (TCNE = tetracyanoethylene) is one component of well-known organic magnets with ferromagnetism up to room temperature. TCNE has a strong electron affinity that facilitates chemical bond formation and charge transfer with metals. We use scanning tunneling microscopy and spectroscopy to study single TCNE molecules on Cu(111) and Cu(100) surfaces. On Cu(111), we find that TCNE can be reversibly switched among three configurations via a controlled voltage pulse. We determine the adsorption sites for these configurations by co-adsorbing CO molecules, which are well known to adsorb atop Cu atoms. We believe these states represent different adsorption configurations and charge states. One of the configurations shows a strong Kondo resonance at low temperature; spectroscopic imaging indicates that this state is strongly localized at the corners of the TCNE molecule. Several features symmetric about V=0 suggest a convolution of the Kondo density of states with inelastic electron tunneling spectroscopy of vibrational modes.

http://www.physics.ohio-state.edu/~jgupta

3NSF CAREER (DMR-0645451)

8:12AM H15.00002 Spin-Electric Coupling in Molecular Magnets

MIRCEA TRIF, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, FILIPPO TROIANI, DIMITRIJE STEPANENKO, DANIEL LOSS, BASEL/MODENA COLLABORATION — We study the triangular antiferromagnet Cu3 in external electric fields, using symmetry group arguments and a Hubbard model approach. We identify a spin-electric coupling caused by an interplay between spin exchange, spin-orbit interaction, and the chirality of the underlying spin texture of the molecular magnetic state. The dispersionless excitation with characteristic intensity modulation is observed at $\hbar \omega = 7.8 \text{ meV}$ at low temperature. The neutron cross section is

8:24AM H15.00003 Magnetic excitation in artificially designed oxygen molecule molecule

TAKATSUGU MASUDA, International Schools of arts and sciences, Yokohama city university, SATOSHI TAKAMIZAWA, KAZUMA HIROTA, MASAAKI OHBA, SUSUMU KITAGAWA — We performed inelastic neutron scattering experiment to study magnetic excitation of O2 molecules adsorbed in microporous compounds. The dispersionless excitation with characteristic intensity modulation is observed at $\hbar \omega = 7.8 \text{ meV}$ at low temperature. The neutron cross section is explained by spin dimer model with intradimer distance of 3.1 Å Anomalous behaviour in the temperature dependence is discussed in the context of enhanced magnetoelasticity in the soft framework of O2 molecule.
8:36AM H15.00004 Influence of the Dzyaloshinskii-Moriya exchange interaction on quantum phase interference of spins, WOLFGANG WERNSDORFER, CNRS, Institut Neel, T.C. STAMATATOS, G. CHRISTOU, Dept. of Chemistry, Univ. of Florida, Gainesville, CNRS, INSTITUT NEEL, GRENOBLE COLLABORATION, DEPT. OF CHEMISTRY, UNI. OF FLORIDA, GAINESVILLE COLLABORATION — Magnetization measurements of a Mn_{12}mda wheel single-molecule magnet (SMM) with a spin ground state of S = 7 show resonant tunneling and quantum phase interference, which are established by studying the tunnel rates as a function of a transverse field applied along the hard magnetization axis. We show how the Dzyaloshinskii-Moriya (DM) exchange interaction can affect the tunneling transitions and quantum phase interference of a SMM. Of particular novelty and importance is the phase-shift observed in the tunnel probabilities of some transitions as a function of the DM vector orientation. Such observations are of importance to potential applications of SMMs that hope to take advantage of the tunneling processes that such molecules can undergo.

8:48AM H15.00005 Coupling between molecular spin cluster qubits, MARCO AFFRONTE, CNR-INFM-S3 — Supramolecular chemistry enables nanoscale engineering of scalable structures, by introducing controlled interactions between well defined molecular building blocks. The ability to assemble weakly-interacting subsystems is a prerequisite for implementing quantum-information processing (QIP) and generating controlled entanglement. In recent years, molecular nanomagnets (MNNs) have been proposed as suitable candidates for the qubit encoding and manipulation. In particular, antiferromagnetic Cr7Ni rings at low temperature behave as effective spin-1/2 systems and exhibit long decoherence times. Here we show that these rings can be linked to each other through supramolecular functional groups, which allow an extensive tuning of the coupling between their spins. We demonstrate that maximally entangled states can be deterministically generated in tripartite supramolecular assemblies, formed by two Cr7Ni rings and a Cu ion, by simulating the system’s time evolution under the effect of realistic microwave pulse sequences (under consideration NanoTechnology).

9:00AM H15.00006 High Resolution Neutron Scattering Studies of Spin Excitations in the 2D Singlet Ground State Systems of SrCu2(BO3)2, SrCu(2-x)Mg(x)(BO3)2 and Sr(1-x)La(x)Cu2(BO3)2, SARA HARAVIFARD, SARAH DUNSIGER, BRUCE GAULIN, HANNA DABKOWSKA, Department of Physics and Astronomy, McMaster University, Hamilton, ON, Canada., MARK TELLING, TOBY PERRING, Rutherford Appleton Laboratory, ISIS Pulsed Neutron Facility, Didcot, Oxford, United Kingdom., SAMIR EL SHAWISH, J. Stefan Institute, Ljubljana, Slovenia., JANEZ BONCA, Faculty of Mathematics and Physics, University of Ljubljana, Ljubljana, Slovenia. — SrCu2(BO3)2 is a quasi-2D quantum spin system known to possess a collective singlet ground state and a realization of the Shastry-Sutherland model. One aspect of the study of SrCu2(BO3)2 for which there is a little information is the influence of impurities on the nature of the singlet ground state. There is much interest in such studies due to the remarkable phenomena associated with doping other quasi-2D copper-oxide quantum magnets with high-T superconductivity. Here we report high resolution time-of-flight neutron scattering studies of single crystals of doped SrCu(2-x)Mg(x)(BO3)2 and Sr(1-x)La(x)Cu2(BO3)2 and compare these results to the pure SrCu2(BO3)2 neutron scattering measurements. Particular emphasis is placed on the lifetimes of one-triplet excitations as well as the existence of in-gap spin excitations in the presence of Mg and La impurities.

9:12AM H15.00007 Entanglement Perturbation Theory for Antiferromagnetic Heisenberg Chains, LIHUA WANG, SUNG CHUNG, Western Michigan University — We use a novel method, Entanglement Perturbation Theory (EPT) to solve the Heisenberg chain comprehensively for both spin 1/2 and spin 1. A variety of quantities for xxx model and xxz model are calculated, including the ground state energies, the spin-spin correlation functions, and the first excited state energies relevant to a phase transition. EPT allows us to calculate systems with nearly one thousand sites and obtain spin-spin correlation functions over hundreds of sites with unprecedented accuracy. The successful application of EPT to the Heisenberg model shows that it is simple, general and exact for macroscopic quantum systems with translational symmetry.

9:24AM H15.00008 MagnetoElectric Coupling in a Quantum Spin Ladder1, JESSICA WHITE, JANICE MUSFELDT, University of Tennessee, SCOTT CROOKER, JOHN SINGLETON, ROSS MACDONALD, Los Alamos National Laboratory, CHRIS LANDEE, MARK TURNBULL, Clark University, HANS CHRISTEN, Oak Ridge National Laboratory — We investigated the optical properties and magnetization of (2,3-dmpyH)2CuBr3, an antiferromagnetic quantum spin ladder with strong rail interactions. It is similar to the copper oxides, yet its modest exchange interactions allows it to be saturated at 29 T, whereas copper oxides require a much higher field. In the end, we were able to see that the field dependent integrated absorption difference tracks the magnetization, demonstrating that the structure is sensitive to the ferromagnetic transition.

1This work is supported by the National Science Foundation

9:36AM H15.00009 Valence-Bond Monte Carlo Study of Random-Singlet Phase Formation, HUAN TRAN, NICHOLAS BONESTEEL, Department of Physics and NHMFL, Florida State University — In valence-bond Monte Carlo (VBMC) the ground state of a quantum spin system is sampled directly from the valence-bond (VB) basis — a useful basis for visualizing the properties of singlet ground states. For example, the ground state of the uniform AFM spin-1/2 Heisenberg chain is characterized by strongly fluctuating bonds with power-law length distribution, while in the random-singlet phase (RSP) of a random Heisenberg chain these bonds, while still having a power-law length distribution, lock into a particular VB state on long length scales. We use VBMC to directly probe the formation of a RSP by calculating both the average number of bonds n_L leaving a block of L spins (the VB entanglement entropy) and its fluctuations, σ^2_n_L = ⟨(n_L^2)⟩−⟨n_L⟩^2. For the uniform chain they have been calculated exactly to and shown to grow logarithmically with L — signaling the strong bond fluctuations. For random chains while n_L grows logarithmically with L, we find σ^2_n_L saturate for large L, signaling the “freezing” of the bonds into a particular random singlet state.

1A. Sandvik, PRL 95, 207203 (2005).

9:48AM H15.00010 Quantum Monte Carlo simulations of dynamical behavior for gapped spin chains1, ZHAOXIN XU, JUANA MORENO, Louisiana State University, MARK JARRELL, Louisiana State University and University of Cincinnati — We study the dynamical properties of spin-1 antiferromagnetic chains and spin-1/2 ferromagnetic-antiferromagnetic bond alternating chains. We calculate their dynamical structure factors using quantum Monte Carlo simulations combined with the Maximum Entropy Method. We focus on the finite temperature dynamical behavior and impurity effects on these gapped spin chains. We also discuss the connection between our results and recent neutron scattering experiments.

1This work was supported by the National Science Foundation through OISE-0730290, DMR-0548011, and DMR-0706379.
The wavelength-independence and the weak constraints on angular alignment and position of the circular obstacle make Poisson's spot a promising candidate for experiments to be realized with neutral matter waves. In this paper we report the observation of Poisson's Spot using a beam of neutral deuterium molecules.

Bergen, Norway — In the Poisson-Spot experiment, waves emanating from a source are blocked by a circular obstacle. Due to their positive on-axis interference, a single spot is observed on a screen placed at a sufficient distance from the source. The spot’s visibility reveals important information on the properties of the examined particles, such as their mass and polarizability.

Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFGANG E. ERNST, Graz University of Technology, Austria, GIANANGELO BRACCO, University of Genova, Italy, HENRY I. SMITH, Massachusetts Institute of Technology, USA, BODIL HOLST, University of Massachusetts Institute of Technology, USA, HERBERT REINGRUBER, KATRIN FLADISCHER, WOLFWA...
8:24AM H16.00003 The Two-Mode Approximation in a Realistic Bose-Josephson Junction in a 85Rb/87Rb BEC Mixture. JEFFREY HEWARD, MARK EDWARDS, Georgia Southern University, CHARLES CLARK, NIST — We have studied the behavior of an experimentally realistic Bose-Einstein condensate (BEC) mixture subjected to a double-well potential. The mixture studied consists of 85Rb and 87Rb held in an optical trap with an external magnetic field that enables tuning of the 85Rb–87Rb scattering length. This system, without the external double-well potential, has been implemented at JILA [S.B. Papp, et al, Phys. Rev. Lett. 101, 040402 (2008)]. A double-well potential can be added to this system by applying a pair of lasers as was done in a previous experiment for single condensates [M. Albiez, et al, Phys. Rev. Lett. 95, 010402 (2005)]. We have used the Variable Tunneling Model (VTM) within the two-mode approximation to search for novel condensate mixture behavior in this experimentally accessible system. Possible behaviors include Bose-Josephson oscillations with both swapping and non-swapping modes and macroscopic quantum self-trapping with zero and pi modes as described in a recent paper [I. Satija, et al, arXiv:0811.1921v1 [quant-ph]]. We compare the behavior as predicted by the two-mode VTM with the solution obtained by integrating the coupled Gross-Pitaevskii equations. We propose some new experiments designed to observe these novel phenomena.

8:36AM H16.00004 Spin-orbit coupled Bose-Einstein condensates. BRANDON ANDERSON, TUDOR STANESCU, VICTOR GALITSKII, University of Maryland — We consider a Bose-Einstein condensate (BEC) of cold atoms with an internal pseudo-spin-1/2 degree of freedom that is coupled to momentum. The pseudo-spin degree of freedom emerges from the trapped multi-level atoms moving in the presence of spatially modulated laser fields. Within a so-called tripod scheme, the atom-laser interaction generates a pair of degenerate dark states. Upon adiabatically projecting onto the dark states subspace, an effective Hamiltonian emerges with a spin-orbit coupled pseudo-spin-1/2 degree of freedom. For a symmetric, Rashba-type spin orbit interaction the ground state of the pseudo-spin space is continuously degenerate along a circle in momentum space and may lead to many-body states with nontrivial topological properties. We investigate the Rashba-type spin-orbit BEC in the presence of weak density-density interactions.

8:48AM H16.00005 Spin Squeezing in Spinor Condensates. SABRINA LESLIE, JAY SAU, MARVIN COHEN, DAN STAMPER-KURN, Physics Dept, UC Berkeley — Spin squeezing in spinor condensates enables the control of quantum spin fluctuations in a fascinating multi-mode system. Further, it provides a coherent spin system characterized by sub-shot-noise spin fluctuations, with applications towards sensitive spatially-resolved magnetometry. With the application of appropriate unitary transformations, we show that one may manipulate the spin fluctuations atop an arbitrary F=1 coherent state, and in so doing prepare an arbitrary F=1 spin squeezed state. Taking into account experimental limitations to spin squeezing such as atom loss and nonlinear interactions in the condensate, we find that one may achieve roughly 17 dB of spin squeezing in the single mode regime and 10 dB of spin squeezing in the multi mode regime, for reasonable experimental parameters.

9:00AM H16.00006 Squeezing and entanglement in a Bose-Einstein condensate. CHRISTIAN GROSS, JEROME ESTEVE, STEFANO GIOVANAZZI, ANDREAS WELLER, MARKUS OBERTHALER — We report on the observation of spin squeezing and entanglement in a Bose-Einstein condensate trapped in double well and periodic potential [1]. The measurement of two conjugate variables - atom number difference and relative phase between adjacent sites - allows a direct connection to the presence of entanglement. The observations indeed confirm that entanglement is present even at finite temperature. The observed coherent spin squeezing of 3.8 dB implies that a usable quantum resource has been generated which is directly applicable to overcome the standard quantum limit of atom interferometry. The limitations due to experimental imperfections, finite temperature and three body loss will be discussed in detail. Latest results on spin squeezing using hamiltonian dynamics of internal states are presented. [1] J. Esteve, C. Gross, A. Weller, S. Giovanazzi and M. K. Oberthaler: Nature 455, 1216-1219.

9:12AM H16.00007 Creation of resilient entangled states and a resource for measurement-based quantum computation with optical superlattices. ANDREAS NUNNENKAMP, Departments of Physics and Applied Physics, Yale University, PO Box 208120, New Haven, CT 06520, USA, BENOIT VAUCHER, DIETER JAKSCH, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, UK — We investigate how to create entangled states with ultracold bosonic atoms trapped in optical lattices by dynamical manipulation of the shape of the lattice potential. We consider a period-two superlattice that allows both the splitting of each site into a double-well potential and also the variation of the height of the potential barrier between the sites. We show how to use this array of double-well potentials to entangle neighboring qubits encoded on the Zeeman levels of the atoms, without using the different vibrational states of the atoms. Finally, we present a method of realizing a Bell-pair encoded cluster state, a resource for measurement-based quantum computing which remains resilient to collective dephasing noise throughout the computation [NJP 10, 023005 (2008)].

9:24AM H16.00008 ABSTRACT WITHDRAWN

9:36AM H16.00009 Numerical Model of Polariton Dynamics in GaAs Quantum Well-Microcavity Structures. VINCENT HARTWELL, DAVID SNOKE, RYAN BALILI, University of Pittsburgh — Recent experimental results from GaAs quantum well-microcavity structures show evidence for Bose-Einstein condensation of polaritons. A main indicator of this is a large accumulation of polaritons near k=0 above a critical density threshold. The polariton gas is never in complete equilibrium, however. To model the system, we therefore cannot use an equilibrium model for the momentum distribution; instead, we have developed numerical methods for solving the quantum Boltzmann equation for the polariton momentum distribution, including the effects of polariton-polariton scattering, polariton-phonon scattering, and polariton scattering with free electrons. The model allows direct comparison to experimental results. An unexpected experimental result which we address in our modeling is that at very low densities, the polariton momentum distribution is invariant and independent of density. At high densities, our numerical model predicts the accumulation of polaritons near k=0 is indeed the result of the boson statistics of the particles, and though it is not in complete equilibrium, it has the characteristics of a “quasicondensate.”

9:48AM H16.00010 Single vortex-antivortex pair in an exciton polariton condensate. GEORGIOS ROUMPOUS, E.L. Ginzton Lab., Stanford University, USA, SVEN HEOFLING, ALFRED FORCHEL, Technische Physik, Universitat Wurzburg, Germany, YOSHIHISA YAMAMOTO, E.L. Ginzton Lab., Stanford University, USA and National Institute of Informatics, Japan — We report the observation of a single vortex-antivortex pair in a two-dimensional exciton polariton condensate. The pairs are evidenced in the time-integrated phase maps acquired using Michelson interferometry. The striped pattern of the sample disorder potential prevents rotation of the pairs, but allows their translational movement.
10:00AM H16.00011 Rabi oscillations in semiconductor multiwave response , MIKHAIL EREMENCHOUK, MICHAEL LEUENBERGER, University of Central Florida — We study the semiconductor response with respect to high intensity resonant excitation on short time scale when the contribution of the Fermi statistics of the electrons and holes prevails. Both the single and double pulse excitations are considered in the framework of asymptotically exact description. For the double pulse excitation we consider the time evolution of the multiwave mixing (MWM) exciton polarization. The main difference between the excitation by a single pulse or by two non-colinear pulses is that the Rabi oscillations of the MWM response are characterized by two harmonics. The operator dynamics governed by the external excitation exhibits three invariant spin classes, which do not mix with the evolution of the system. Two classes correspond to the bright exciton states and one contains all dark states. The dynamics of the classes turn is described by six characteristic frequencies and the Rabi frequencies (RF) are only two of them (one for each bright class). We show that if initially the system is in the ground state then the semiconductor Bloch equation preserves the invariant spin classes thus proving absence of the dark excitons in the framework of this description. We found that due to the mass difference between holes of different kind two additional RF’s, presenting in the operator dynamics, should appear in the evolution of the exciton polarization.

10:12AM H16.00012 Single-atom trajectories of intermittent fluorescence with quantum jumps , PATRICK COLES, ROBERT GRIFFITHS, Department of Physics, Carnegie Mellon University — Understanding the trajectories of single quantum systems is a modern theoretical challenge, given that experiments are no longer restricted to ensemble-averaged dynamics. Here, we present a model for a single 3-level atom driven resonantly on two transitions, resulting in intermittent fluorescence from one transition. The consistent histories formalism provides insight into the intermittent “shelving” process and predicts the distribution of dark periods for a given trajectory. We further predict quantum interference that leads to oscillations in the quantum-jump probability and discuss the possibility of observing these oscillations experimentally.

10:24AM H16.00013 Dynamics and fidelity of entanglement of photons coupled to optical fibers and waveguides , BEREKET BERHANE, Embry-Riddle Aeronautical University — We investigate the time evolution of the quantum mechanical states of photon-modes in optical fibers and waveguides starting from a multipolar coupling of neutral atoms with a quantized electromagnetic field. We apply our results to the propagation of entangled photons in optical fibers and investigate the fidelity of entanglement for various optical fiber lengths. Furthermore, we obtain a quantum input-output formalism in three dimensions and investigate the dependence of coupling and transfer efficiency on the quantum state of the incident photons. We apply our results to the coupling and propagation of entangled photons for applications in quantum memory transfer over optical fibers and waveguides.

10:36AM H16.00014 Quantum fluctuations in small lasers , KAUSHIK ROY CHOUDHURY, STEPHAN HAAS, A.F.J LEVI, University of Southern California — Master equations are used to demonstrate the dominant role of quantum fluctuations in determining the steady-state and transient response of a laser when there is a small number of particles in the system. In this regime, quantum fluctuations are found to suppress the lasing threshold and create a non-Poisson probability distribution for n and transient response of a laser when there is a small number of particles. In this regime, quantum fluctuations are found to suppress the lasing threshold and create a non-Poisson probability distribution for n and transient response of a laser when there is a small number of particles.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H17 GQ1: Focus Session: Semiconducting Qubit Approaches 318

8:00AM H17.00001 Solid state quantum memory using 31P spins in silicon: advantages of hybrid qubit systems , JOHN MORTON, Oxford University — No abstract available.

8:36AM H17.00002 Radio-frequency single-electron transistor coupled to a few-electron double quantum dot1, FENG PAN, JOEL STETTENHEIM, MUSTAFA BAL, MINGYUN YUAN, ALEX RIMBERG, Dartmouth College, VLADIMIR UMANSKY, Weizmann Institute of Science — The radio frequency single-electron transistor (rf-SET) has been shown to be a ultra fast and highly sensitive electrometer, and can be potentially operated close to the quantum noise limit as a qubit readout device [1]. The interplay between the rf-SET electrometer and a two-level system offer an interesting system for study. Here we report our progress on investigating rf-SET's capacitively coupled to few-electron double quantum dots (DQDs). We fabricate lateral-defined DQDs from an AlGaAs/GaAs heterostructure and the rf-SET from superconducting aluminum embedded in a tank circuit. The sensitivity and bandwidth of on-chip rf-SET electrometer can be used to probe DQD operated in the few-electron regime. We have observed coupling between SET and DQD and have optimized our device design to enhance coupling in the few-electron limit. Recent experimental results will be discussed. [1] M. H. Devoret and R. J. Schoelkopf, Nature, 406, 1039 (2000).

1Supported by the NSF and ARO.

8:48AM H17.00003 3D Acoustic Modes, Shot Noise and Strain Displacements in a Radio Frequency Quantum Point Contact1, J. STETTENHEIM, Dartmouth College, M. THALAKULAM, U. Wisconsin-Madison, F. PAN, M. BAL, Dartmouth College, L.N. PFIEFFER, K.W. WEST, Bell/Lucent, A.J. RIMBERG, Dartmouth College — As previously reported, our broadband frequency resolved measurements of shot noise in a radio frequency QPC (RF-QPC) reveal a remarkable frequency dependence absent from theoretical predictions. Based on piezoelectric coupling in GaAs, our data suggest a feedback loop in which shot noise drives resonant acoustic vibrations that in turn create correlations in electron tunneling. The feedback concentrates the initially white noise in a narrow band around the sample’s resonant frequency, allowing shot noise spectrum engineering. We solve for the 3D acoustic modes of our samples, finding close correspondence with measured frequencies. We have determined that the geometry and magnitude of the polarization field selects the acoustic mode excited. As polarization fields and strain displacements are linked in GaAs, we estimate the ultimate mechanical displacement sensitivity of our RF-QPC.

1Supported by the NSF and ARO.
9:00AM H17.00004 Radio-frequency quantum point contact in a silicon/silicon-germanium two-dimensional electron system, MADHU THALAKULAM, CHRISTIE SIMMONS, ERIC SACKMANN, BJORN VAN BAEL, D.E. SAVAGE, MAX LAGALLY, M.A. ERIKSSON, University of Wisconsin-Madison — Radio frequency quantum point contacts (RF-QPC) are sensitive and fast electrometers. The capability to integrate such devices with semiconductor-based quantum dot systems makes them an attractive candidate for fast charge readout, and the increasing interest in spins in group-IV quantum dots motivates the development of such devices in silicon/silicon-germanium two-dimensional electron systems. We report the operation of an RF-QPC fabricated on a silicon/silicon-germanium heterostructure with an on-chip matching network. An on-chip spiral inductor and the capacitance from the bonding pads define the tank circuit. The inductance and capacitance parameters are optimized to achieve a resonant frequency of approximately one GHz. The operation of RF-QPC at milli-Kelvin temperature and the charge readout of a quantum dot system using an RF-QPC will be discussed.

9:12AM H17.00005 Observation of tunnel rates of phosphorus dopants using silicon SETs, H. HUEBL, C.D. NUGROHO, A. MORELLO, C. ESCOTT, A.S. DZURAK, R.G. CLARK, Centre for Quantum Technology, University of New South Wales, Sydney, C. YANG, J.V. DONKELAAR, A. ALVES, D. JAMIESON, Centre for Quantum Computer Technology, University of Melbourne, Melbourne, M.A. ERIKSSON, Department of Physics, University of Wisconsin, Madison, Wisconsin — Charge centres, such as donors in semiconductors, have significant potential for quantum information processing. In silicon, which can be produced nuclear-spin free, phosphorus donors are a prime candidate for implementation of a qubit, due to their long spin coherence times. In this presentation we will discuss a hybrid structure, consisting of implanted phosphorus donors connected by a gate potential in close vicinity to a gate-induced, MOS-based silicon single electron transistor (Si-SET). We study the dual functionality of the nearby Si-SET as a sensitive charge detector as well as a gate-induced electron reservoir. Experimentally, we observe shifts in the position of the Coulomb peaks of the Si-SET corresponding to ~20% of an electron charge. We attribute these shifts to charge transfers between the Si-SET island reservoir and the nearby phosphorus donors. Pulsed voltage spectroscopy on one of these charge transitions allows us to investigate the capture and emission times of a donor resulting in a capture rate of 3000 s^-1 and an emission rate of 1000 s^-1 corroborating expectations from device modelling.

9:24AM H17.00006 Self-Correcting Dynamic Decoupling Pulse Sequences, ALEXEI M. TYRYSHKIN, STEPHEN A. LYON, Princeton University, WENXIAN ZHANG, VIATCHESLAV V. DOBROVITSKI, Ames Laboratory — Dynamic decoupling (DD) techniques employ a series of strong refocusing pulses to combat decoherence in quantum systems. However, each DD pulse is imperfect and thus introduces a small instrumental error; the error can accumulate rapidly upon applying many DD pulses, and this error can destroy the quantum state. We have examined several DD pulse sequences, including CPMG, ZZXX, ZXYX and their concatenated variants, using electron spin resonance (ESR) of donors electron spins in silicon. While all these DD sequences performed comparatively in cancelling the phase noise arising from magnetic field fluctuations, only one sequence (ZXYX) demonstrated the ability to protect an arbitrary coherent state, including X, Y, and Z states in the rotating frame. The other sequences (CPMG and ZZXX) were able to store only one state (Y) while destroying other states (X and Z). The superior performance of ZXYX arises from its internal ability to correct for pulse amplitude errors, the dominant error in these ESR experiments.

9:36AM H17.00007 ABSTRACT WITHDRAWN —

9:48AM H17.00008 Hyperfine tolerant triplet-singlet qubit in rotating double quantum dots, DAVID DRUMMOND, LEONID P. PRIYADKO, KIRILL SHTENGEL, Univ. California, Riverside — We examine the triplet-singlet state of pairs of GaAs single electron quantum dots, in which the singlet and m=0 triplet states represent the logical 0 and 1. Each electron’s spin feels a different magnetic field from the hyperfine coupling to the local nuclei of the GaAs, leading to a relative phase difference between the two electrons, and thus decoherence. Previous methods have delayed decoherence using complicated electrical pulse schemes or nuclear polarization with Overhauser fields, which can only be maintained for short times and require great energy. Instead we propose to eliminate hyperfine decoherence by repeatedly rotating the dots adiabatically, exposing the electrons to the same average magnetic field. In addition, we show that if these rotations are performed repeatedly in a symmetric fashion, the Dresselhaus and Rashba spin-orbit couplings are significantly suppressed. The construction of such a device might also be of interest to topological quantum computers, which depend on similar rotations.

10:00AM H17.00009 Multiple Nuclear Polarization States in a Double Quantum Dot, JEROEN DANON, Delft University of Technology — In a double quantum dot under conditions of electron paramagnetic resonance we have observed multiple stable states of nuclear polarization and also switching between those states. The system exhibited strong hysteretic behavior over a large range of magnetic fields, indicating the dynamical buildup of effective magnetic nuclear fields up to 150 mT. We have explained these findings in the framework of an elaborated theoretical model. The results reported enable applications of this nuclear polarization effect, including manipulation and control of the nuclear fields and possible use of this for improving the electron spin coherence time.

10:12AM H17.00010 Electron spin dephasing by hyperfine-mediated interactions in a nuclear spin bath, LUKASZ CYWINSKI, University of Maryland, College Park, WAYNE M. WITZEL, Naval Research Laboratory, Washington DC, SANKAR DAS SARMA, University of Maryland, College Park — We investigate pure dephasing decoherence (free induction decay and spin echo) of a quantum dot spin qubit interacting with a nuclear spin bath. While for infinite magnetic field the only decoherence mechanism is spectral diffusion due to dipolar flip-flops of nuclear spins, with decreasing B the hyperfine-mediated interactions between the nuclear spins become important. We give a theory [1] of decoherence due to these interactions which takes advantage of their long range nature. For a thermal uncorrelated bath we show that our theory is applicable down to B~10 mT, allowing for comparison with recent experiments on spin echo in GaAs quantum dots [2].


This work is supported by LPS-NSA.

10:24AM H17.00011 Nuclear State Preparation via Landau-Zener-Stückelberg transitions in Double Quantum Dots, HUGO RIBEIRO, GUIDO BURKARD, University of Konstanz — We theoretically model a nuclear-state preparation scheme that increases the coherence time of a two-spin qubit in a double quantum dot. The two-electron system is tuned repeatedly across a singlet-triplet level-anticrossing with alternating slow and rapid sweeps of an external bias voltage. Using a Landau-Zener-Stückelberg model, we find that in addition to a small nuclear polarization that weakly affects the electron spin coherence, the slow sweeps are only partially adiabatic and lead to a weak nuclear spin measurement and a nuclear-state narrowing which prolongs the electron spin coherence. Based on our description of the weak measurement, we simulate a system with up to n=200 nuclear spins per dot and qualitatively explain recent experimental findings. Scaling in n indicates a stronger effect for larger n, also in qualitative agreement with experiments.
10:36AM H17.00012 Electromagnetic fluctuations as a source of decoherence for double quantum dot charge-based qubits, DIEGO VALENTE, Department of Physics, University of Central Florida, FRANK WILHELM, Institute for Quantum Computing, University of Waterloo, EDUARDO MUCCIOLLO, Department of Physics, University of Central Florida — Solid-state quantum dots are strong candidates for the physical realization of qubits. They present the ubiquitous advantage of easier scalability, but also couple rather effectively to external degrees of freedom which lead to decoherence phenomena. One such source of decoherence lays in the electromagnetic fluctuations occurring in the circuits utilized for preparation and measurement of these qubits. Here we investigate these sources of decoherence in double quantum dot charge-based qubit systems. We use effective circuit models and estimates of time correlations of such fluctuations to calculate the energy ($T_1$) and phase ($T_2$) relaxation times introduced into the qubit system. We also present ideas on how to suppress some of the destructive effects of these fluctuations and increase the quality factor for quantum oscillations.

1Supported by: NSF-EMT CCF-0523509 and CCF-0523603.

10:48AM H17.00013 Probing the spin structure of $\nu = 2$ quantum Hall fluid around an antidot, LEE BASSETT, CHRIS FORD, NIGEL COOPER, JONATHAN GRIFFITHS, DAVID ANDERSON, IAN FARRER, GEB JONES, DAVE RITCHIE, University of Cambridge — We experimentally investigate spin and charge excitations in a small closed edge of integer quantum Hall fluid encircling a nano-scale potential island, or antidot (AD), in a two dimensional electron system. Using quantum point contacts to inject and detect spin-polarized currents via edge states, we have measured spin-resolved transport through single ADs at filling factor two. At relatively low magnetic fields (\approx 1T), tunneling between the AD states and higher Landau levels in the bulk produces pairs of Coulomb blockade peaks in conductance above the $2e^2/h$ plateau. These transmission resonances were thought to result from spin-polarized tunneling through individual single-particle AD states (of alternating spin), but our experiments show that, while spin is generally conserved during transport, the tunneling current is not spin-polarized. We interpret these results as signatures of interactions within the AD which result in a separation of the energy scales associated with spin and charge excitations.

Tuesday, March 17, 2009 8:00AM - 10:48AM –
Session H18 DPOLY: Block Copolymer Thin Films I 319

8:00AM H18.00001 Polymer Physics Prize Symposium Break –

8:36AM H18.00002 Analysis of block-copolymer thin film ordering through a moving thermal zone, KEVIN YAGER, NATHANIEL FRÉDIN, RONALD JONES, Polymers Division, National Institute of Standards and Technology — Block-copolymer thin films self-assemble into well-defined structures at the nanometer lengthscale. It has been shown that the morphology, orientation, and degree of order resulting from annealing is sensitive to a variety of preparation parameters, including annealing time and temperature, solvent exposure, substrate surface energy, application of electric fields, etc. A moving thermal zone can also strongly affect the ordering. We have shown that relatively “cold” zone annealing (CZA) conditions (above the glass-transition but well below the disordering temperature) can induce a preferential orientation of the microdomains in thin films. We further analyze this effect by measuring the ordering through the thermal front, using atomic force microscopy and scattering techniques (reflectivity and GI-SAXS), which are combined to quantify the order and 3D orientational distribution. Zone annealing leads to increased grain sizes and substantially faster coarsening kinetics, as compared to oven annealing. Moreover, the evolution of order through the thermal front constrains models which aim to explain the CZA’s ability to induce orientational bias.

8:48AM H18.00003 Neutral Parameter Window for Perpendicularly Oriented Block Copolymer Resists Deposited on Organosilicate Substrates with Tunable Surface Energy, HYOSEON SUH, KOOKHEON CHAR, Seoul National University, HUIMAN KANG, PAUL F. NEALEY, University of Wisconsin — Balancing the interfacial interactions of a block copolymer (BCP) with a substrate as well as the free surface can induce the perpendicular orientation of microdomains, allowing the BCP films to serve as templates for nanofabrication. However, it is known that such orientation of microdomains is quite sensitive to the film thickness. In this presentation, we investigated the effect of film thickness on the orientation of microdomains in lamellae-forming P(S-b-MMA) thin films placed on thermally cured organosilicate (OS) substrates. For the film thickness of a P(S-b-MMA) ranging from 1 L$_0$ up to 2.5 L$_0$, we varied the surface energy of the OS substrate around the value close to the enthalpically neutral condition by controlling the substrate cure temperature. We will demonstrate the origin of the observed thickness effect by taking into account the increase in surface area at the free surface when P(S-b-MMA) films make holes or islands depending on the incommensurable conditions of the BCP film. This analysis allows us to define a more accurate neutral window for the P(S-b-MMA) in terms of both substrate surface energy and BCP film thickness.

9:00AM H18.00004 Effect of Surface Energies on Block Copolymer Thin Film Phase Behavior, JULIE LAWSON, MICHAEL BANEY, THOMAS EPPS, University of Delaware — The development of block copolymer materials for future nanotechnologies requires an understanding of how surface energetics affect block copolymer thin film phase behavior. In this work, we use combinatorial methods to study these effects and to identify transitions in thin film phase behavior and microstructure orientation. Surface energy gradients were created using a vapor deposition technique developed by our group in which cross-diffusion of functionalized chlorosilanes under dynamic vacuum results in a linear gradient in surface energy on a silicon substrate. These gradients were characterized using X-ray photoelectron spectroscopy (XPS) and contact angle measurements. We then cast a thin film of block copolymer on the modified substrates using a flow coating technique. Finally, we used thermal and solvent annealing conditions to affect the surface energy at the free surface. The surface morphology of the films was examined with atomic force microscopy (AFM), and morphological changes across the gradient were found.

1National Science Foundation DMR 0645586, National Science Foundation Graduate Research Fellowship

9:12AM H18.00005 Systematic tunability of self-assembled block copolymer patterns, YEON SIK JUNG, CAROLINE ROSS, Massachusetts Institute of Technology — The morphology and length scale of diblock copolymers (BCPs) are determined by the chain lengths, and therefore to obtain different geometries and feature sizes, polymers with different chain lengths or BCP/homopolymer blends have been employed. Here, we report on the solvent vapor induced tunability of pattern dimension and morphology of thin films of polystyrene-polydimethylsiloxane (PS-b-PDMS) BCPs, which provide robust patterns with exceptionally good ordering due to their large interaction parameter. Vapor pressure can control the interfacial interaction between the two blocks, and a mixed solvent can manipulate the effective volume fraction of each block. We show both coupled and independent control of the microdomain size and the periodicity by changing the vapor pressure and the mixing ratio of a selective (heptane) and a partially selective (toluene) solvent. We also demonstrate the transformations from spheres to cylinders and from cylinders to perforated lamellar structures by increasing the portion of selective solvent in the vapor. These results are supported by a theoretical model.

9:24AM H18.00006 Solvent annealing of Micropatterned PS-b-PEO copolymer films1. TAE HEE KIM, HIMADRI ACHARYA, HEE JUNE JOENG, CHEOLMIN PARK, Yonsei University — Solvent annealing of block copolymer thin films have been known as an effective way to control both orientation of microdomains with respect to the surface and their registration into a well ordered periodic lattice structure. We have recently demonstrated hierarchically ordered microdomains in a thin poly(styrene-b-ethylene oxide)(PS-b-PEO) film combined with microcontact printing. The solvent annealing gave rise to well ordered spherical PEO microdomains in large area by the confined dewetting of thin PS-b-PEO films which had been micropatterned on chemically modified surface during solvent annealing. In this presentation, we intentionally prepare a micropatterned dewet film of PS-b-PEO by spincoating a block copolymer solution on a topographic PDMS pre-pattern. Convex lens shaped spherical caps of PS-b-PEO individually located on each PDMS mesa were successfully transferred to a Si substrate by a conventional transfer printing technique. We investigate the effect of solvent on not only film wettability but also formation of hierarchical nanostructures.

3This research was supported by National Research Program for Memory Development and “SYSTEM2010” project sponsored by Korea Ministry of knowledge and economy and Samsung Electronics, Co., Ltd.

9:36AM H18.00007 Transition Behavior of Block Copolymer Thin Films. DU YEOL RYU, CHANGHAK SHIN, HYUNJU AHN, JUNE HUH, Yonsei University, Korea, KWANG-WOO KIM, Pohang Accelerating Laboratory, Korea, THOMAS RUSSELL, University of Michigan — We examine the transition behavior of thin films of diblock copolymers at the substrate/polymer interface. We employ the modified theory for bilayer model with surface capillary waves on simple viscoelastic liquid films. The viscosity obtained in this study is compared with that from rheology measurements for bulk. We found that the PDMS-rich layer near the surface appears at the temperature higher than the glass transition temperature. We apply the modified theory for bilayer model to thin films and show that the order to disorder transition, when the enthalpic term of free energy of mixing is equal to the entropic term. In thin films, interactions at the substrate/polymer and polymer/air interfaces influence this free energy balance, resulting in a change in the transition behavior. Here, we report on the transition behavior of BCP thin films. The thickness dependence of the transition temperature shows that interfacial interactions enhance the orientation of the lamellar microdomain parallel to the film surface even in 40L0 in thickness, where L0 is the equilibrium period of the BCP in the bulk. In thin film geometry, this phenomenon can be attributed to the fact that a preferential interaction of one component with the substrate leads to an amplification of a periodic variation in the composition and a shift of transition temperature.

9:48AM H18.00008 Thin Film Morphology of Diblock and Triblock Copolymers with Bulk Order-Order Transition (OOT). K.E. SOHN, R.C. COFFIN, G.C. BAZAN, E.J. KRAMER, UCSB, K. KOJIO, Nagasaki, B.C. BERRY, A. KARIM, NIST, M. SPRUNG, J. WANG, ANL — The thin film morphology of SEB and SEBS block copolymers that have an OOT in the bulk from cylinders to spheres as the annealing temperature is increased was studied as a function of increasing film thickness using AFM and GISAXS. For both SEB and SEBS, the morphological transition is the same no matter if the film is annealed above or below the bulk OOT. The SEB morphology is governed by the free energy penalty due to chain stretching, showing spheres when the film thickness is less than that of a monolayer of cylinders. The cylindrical morphology dominates when the film thickness is larger than two monolayers of cylinders. The SEBS morphology is governed by the free energy penalty due to loops of the midblock at the surface. Spheres require a lower fraction of midbloks to loop at the surface than cylinders, therefore spheres pay a lower free energy penalty due to chainlooping and were found for all film thicknesses studied (up to ~100nm).

10:00AM H18.00009 UV-Induced Order-to-Order Transition (OOT) in Thin Films of Supramolecular Diblock Copolymer Assemblies Containing 2-(4'-Hydroxyphenylazo)benzoic Acid. WEI CHEN, JIA-YU WANG, XINYU WEI, ANNA BALAZS, THOMAS RUSSELL — Long-range lateral ordering and orientation in block copolymer thin films, which are highly desired for applications requiring addressability, as in magnetic storage, can be obtained in a controlled way via a one-dimensional order-to-order transition (OOT) in microphase separated structure. The photoinitiation and photolysis of benzene results in volume changes that, when integrated into copolymers, can bring about phase transitions that, in turn, by sweeping the light across a surface, will promote long-range lateral ordering, similar to zone-refinement process used to produce large single crystals. We investigated UV-induced OOT in the supramolecule-assembled thin films of 2-(4'-hydroxyphenylazo)benzoic acid and polystyrene-block-poly(2-vinylpyridine) diblock copolymer. Grazing incidence small angle X-ray scattering demonstrated that phase transition from lamellae to hexagonally packed cylinders occurred at 150 °C after UV radiation for 1 hour due to a significantly enhanced interfacial fluctuations induced by photoisomerization as evidenced by X-ray Reflectivity. This suggested that UV light can be utilized to control OOT in the supramolecule-assembled thin films and, hence, to fabricate long range ordered nanostructures, and even smart responsive surfaces.

10:12AM H18.00010 Dilute Micelle Arrays in Block Copolymer Thin Films. JOHN PAPALIA, RICHARD REGISTER, Princeton U., DOUGLAS ADAMSON, U. Connecticut, PAUL CHAIKIN, NYU — Thin films of sphere-forming block copolymers are attractive templates for surface patterning and nanofabrication. While the areal density of spheres (micelles) can be adjusted through the diblock’s molecular weight, sparse micelle arrays are quite difficult to achieve. Instead, we blend the diblock with matrix homopolymer in the “dry brush” regime, which eliminates the “terracing” (island/ hole formation) present in films of the neat diblock. Furthermore, by choosing a system where the sphere-forming block wets the substrate and/or free surface, we control the areal density of micelles by stepwise dilution with PS matrix homopolymer dilution, by using the film thickness as the control parameter rather than the blend ratio. Specifically, we employ a polystyrene-poliosoponoe diblock (PS/PI blocks of 68/12 kg/mol) blended with PS homopolymer; the PI block wets both the free surface and the SiOx substrate. For sufficiently thin films (<60 nm for 50 wt% homoPS), all the block copolymer goes to form brush-like layers at the two surfaces, yielding no micelles. For thicker films, sufficient block copolymer remains to form spherical microdomains between the brushes; the areal density of micelles can be continuously tuned via the film thickness. We evaluate this approach by preparing a film with a thickness gradient, and apply a simple model to the measured areal densities of micelles.

10:24AM H18.00011 Surface Dynamics of Segregation Layer in Blockcopolymer Films1. SANG- HOON SONG, WONSUK CHA, Sogang University, Korea, ZHANG, JIANG, SURESH NARAYANAN, Advanced Photon Source, ANL, ADRIAN RUEHM, Max Planck Institute for Metal Research, Germany, SUNIL K. SINHA, Univ. of California, San Diego, HYUNJUNG KIM, Sogang University — We have investigated the surface dynamics of supported block copolymer films of poly(styrene)-b-poly(dimethylsiloxane) (PS-b PDMS) in the spherical phase, i.e., PDMS cores surrounded by PS shells by x-ray photon correlation spectroscopy (XPCS) in grazing angle geometry. The experiment was performed at the beamline 8ID-I in Advanced Photon Source. We found that the PDMS-rich layer near the surface appears at the temperature higher than the glass transition temperature. We applied the modified theory for bilayer model to thin films and show that the order to disorder transition, when the enthalpic term of free energy of mixing is equal to the entropic term. In thin film geometry, this phenomenon can be attributed to the fact that a preferential interaction of one component with the substrate leads to an amplification of a periodic variation in the composition and a shift of transition temperature.

1This work was supported by Korea Research Foundation, Korea Science & Engineering Foundation, and Seoul Research and Business Development Program (10816).

10:36AM H18.00012 Block Copolymer Brushes1. MARK MATSEN, University of Reading — Using self-consistent field theory (SCFT), we examine dry brushes of AB diblock copolymer, where the B ends are uniformly graftied to a planar substrate. Four different morphologies are predicted, which are conveniently described as the uniform, stripe, hexagonal, and inverted hexagonal phases on the basis of the patterned formed at the air surface by the A-rich domain. Phase diagrams are calculated for different grafting densities and for different A-segment surface affinities. In contrast to unanchored diblock-copolymer films, the brush system has a much greater tendency to form chemically-patterned surfaces.

1Sponsored by EPSRC (grant no. EP/F029616/1)
The obtained values are in good agreement with the dynamic heterogeneity length estimated by 4 dimensional NMR for the main structural relaxation. Thus the relative timescale of the relaxational process by altering the polymer network structure is shown to directly influence the Case II front propagation velocity and the nature of the observed transport behavior.

9:24AM H19.00006 On the Nature of Gas Transport of Ethylene Vinyl Alcohol Copolymers
SERGEI NAZARENKO, JUSTIN BRANDT, BRIAN OLSON, University of Southern Mississippi, ALEXANDER JAMIESON, Case Western Reserve University — Historically, all the approaches describing gas diffusion in polymers can be roughly divided in two categories, based on free volume models and the activation molecular models, which take into account the cooperative penetrant-polymer chain motions, chain rigidity and intermolecular forces. Although gas transport characteristics exhibit a general correlation with free volume, alone free volume can not adequately describe gas barrier. The chain rigidity and the strength of intermolecular interactions are two additional important factors which are manifested via activation energy. The main objective of this work was to develop fundamental understanding of oxygen transport in a broad range of EVOH copolymers as it is related to free volume characteristics probed by positron annihilation lifetime spectroscopy and hydrogen bonding interaction.
elastic modulus is the inverse of the decaying characteristic relaxation time. Parameter of the isothermal ripening process is the “ripening time”, scaling function with two pronounced powerlaw regions, a fast ripening process ($G_t$), scaling relations for the slow ripening of an out-of-equilibrium model colloidal solid that consists of clay particles that swell and exfoliate into randomly oriented hardening in bidisperse glasses and its relation to microscopic conformational changes. The mixtures contain chains of very different lengths but equivalent topological constraints. Unlike related algorithms, the chain shortening has little effect on the craze structure, allowing the entanglements to be followed in real space, as well as along chains. CRETA is applied to molecular simulations of crazing using a coarse-grained bead-spring polymer model. The number of beads in each chain $N$ and the entanglement length $N_e$ are varied. Our results show that entanglements do not act like fixed chemical crosslinks. There is a systematic loss in entanglements during craze formation that does not occur when chains are deformed affinely and is nearly independent of $N/N_e$. The role of chain length, $N$, interchain friction and other parameters in determining the degree of entanglement loss is discussed.

We gratefully acknowledge support of the NSF-IGERT fellowship program

10:00AM H19.00009 Dynamics of a polymer nanocomposite during active deformation, ROBERT RIGGLEMAN, GREGORY TOEPPEWEIN, JUAN DE PABLO, HAU-NAN LEE, M. D. EDGER, University of Wisconsin, Madison — Recent molecular simulation and experimental studies have explored the effects of stress on the dynamics of polymer glasses and both have demonstrated that relaxation times can decrease by more than two orders of magnitude. However, many questions on the origins of the changes in the dynamics remain unaddressed. In this study, we have performed extensive molecular dynamics and Monte Carlo simulations of a polymer glass and a polymer nanocomposite undergoing active deformation. We measure the dynamics during both constant stress and constant strain rate deformations and provide a detailed comparison of the two modes of deformation. The nanoparticles impart mechanical reinforcement onto the polymer, requiring larger stresses to achieve the same deformation. In both systems, the dynamics correlate very well with the instantaneous strain rate whether we deform at constant stress or constant strain rate. Additionally, we explore the effects of each mode of deformation on the potential energy landscape and find qualitatively different behaviors when we deform at constant stress versus constant strain rate. Finally, we provide a brief comparison of our simulation results to recent experiments and demonstrate that the simulations are capable of reproducing all of the behaviors observed in the experiments.

10:12AM H19.00010 Rheological Scaling Relation for an Out-of Equilibrium Colloidal Solid1, H. HENNING WINTER, University of Massachusetts Amherst, X. WANG, G. XUE, Nanjing University, China, P. SUN, Nankai University, China — We explore scaling relations for the slow ripening of an out-of-equilibrium model colloidal solid that consists of clay particles that swell and exfoliate into randomly oriented clay sheets through the action of end-functionalized (“sticky”) polymer molecules. A freshly mixed sample quickly forms a sample-spanning network structure that gradually approaches its equilibrium. The ripening process accelerates at elevated temperature. After rescaling (Rheol Acta 45:331-338, 2006), the complex modulus data $G'(\omega)$, $G''(\omega)$ from time-resolved mechanical spectroscopy (Rheol Acta 33:385-397, 1994) shows that, surprisingly, the growth function of the elastic modulus is the inverse of the decaying characteristic relaxation time. Parameter of the isothermal ripening process is the “ripening time”, $t_r$. A single scaling function with two pronounced powerlaw regions, a fast ripening process ($\sim t_r^{-2}$) followed by slow ripening ($\sim t_r^{-1/2}$), defines the state of ripening and projects the time necessary to reach equilibrium.

1 NSF support through CBET-0651888.

10:24AM H19.00011 Strain Hardening in Bidisperse Polymer Glasses, MARK O. ROBBINS, Johns Hopkins University, ROBERT S. HOY, Materials Research Laboratory, University of California, Santa Barbara — The connections between glassy and rubbery strain hardening have been a matter of great controversy in recent years. Recent experiments and our earlier simulations have suggested that the hardening modulus $G_r$ is proportional to the entanglement density in glasses, as it is to the crosslink density in rubbers. In this work we present more extensive studies of strain hardening in bistable glasses and its relation to microscopic conformational changes. The mixtures contain chains of very different lengths but equivalent chemistry. $G_r$ does not scale simply with the entanglement density. Instead it obeys a simple mixing rule, with $G_r$ equal to the volume fraction weighted average of the moduli of the two pure components. As in recent studies of monodisperse systems (R. S. Hoy and M. O. Robbins, Phys. Rev. Lett. 99, 117801 (2007)), the stress is directly correlated to the degree of chain orientation. Chains of a given length undergo almost the same degree of alignment in pure systems and mixtures, explaining why the mixing rule applies. The connection to recent analytic theories by K. Chen and K. S. Schweizer (PRL, in press) will be discussed.

10:36AM H19.00012 A Model of Glassy Polymers that Includes both Spatial and Temporal Fluctuations, GRIGORI MEDVEDEV, JAMES CARUTHERS, Purdue University — Glass forming polymers near and below $T_g$ are dynamically heterogeneous as has been found via a number of experimental techniques, where the dynamic heterogeneity is the probable cause of the non-exponential decay of the orientation correlation function of probe molecules embedded in polymer matrix as well as “breaking” of the Stokes-Einstein relations for rotational and translational diffusion. Although dynamic heterogeneity in glassy polymers is well established, constitutive models for describing the mechanical behavior employ quantities that ignore fluctuations. Consequently, the mechanical implications of dynamic heterogeneity are largely unexplored. In this talk we report on a finite element type model, where the local relaxation times in the material experience fluctuations, i.e. both the temporal and spatial nature of the fluctuations is explicitly acknowledged. The stochastic force between neighboring domains is assumed to be uncorrelated; however, since neighboring domains tile space, there is spatial and temporal correlation in the stochastic response of the system. The mechanical response of the sample under different deformation histories, including constant strain rate tensile and compressive loading as well as creep under constant load, will be presented.
polymers within the film greatly extends the pH range of stable electroactivity. Immobilization of polyaniline within a polymer acid matrix retards dopant diffusivity and reduces proton mobility. The preservation of local acidic conditions previously reported polyaniline systems. In comparison, polyaniline that is doped with small-molecule acids loses its electroactivity in solutions beyond pH 4. We studied the stability of polyaniline that is template synthesized on poly(2-acrylamido-2-methyl-1-propanesulfonic acid) as a function of pH. Transitions between biosensor and organic electrochemical transistor devices. For many conducting polymers, however, stable electrochemical activity often demands restrictively side of the chain to the other. This causes bending in alternating directions, leading to a sinuosoidal shape, while maintaining a straight chain axis on average.

Since PPY and PANI can change from a coil to a straight rod, these polymers can achieve strains about an order of magnitude higher than PA. This work was supported by Honda R&D Co., Ltd.

**Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H20 DPOLY: Electrically and Optically Active Polymers**

**8:00AM H20.00001 Polymer Physics Prize Symposium Break**

**8:36AM H20.00002 Soliton and polaron induced 3D conformational changes in conjugated polymers**

**8:48AM H20.00003 Conjugated Polymer based sensor for detecting explosives such as RDX (1,3,5-Trinitrohydro-1,3,5-triazine)**

**9:00AM H20.00004 Charge-transfer excitons in strongly coupled organic semiconductors**

**9:12AM H20.00005 Highly Conductive Polymer Films by Post-Processing Solvent Annealing and Their Broad Applications in Organic Electronics**

**9:24AM H20.00006 Electrochemical Stability of Poly(aniline) Beyond pH 9**

1 Corresponding author

1 This work was supported by Honda R&D Co., Ltd.
9:36AM H20.00007 Quadratic Electro-optic Effect in a Novel Nonconjugated Conductive Polymer, iodine-doped Polynorbornene. ANANTHAKRISHNAN NARAYANAN, MRINAL THKUR, Photonic Materials Research Laboratory, Auburn University, AL. — Quadratic electro-optic effect in a novel nonconjugated conductive polymer, iodine-doped polynorbornene has been measured using field-induced birefringence at 633 nm. The electrical conductivity of polynorbornene increases by twelve orders of magnitude to about 0.01 S/cm upon doping with iodine. The electro-optic measurement has been made in a film doped at the medium doping level. The electro-optic modulation signal was recorded using a lock-in amplifier for various applied ac voltages (4 kHz) and the quadratic dependence of the modulation on the applied voltage was observed. A modulation of about 0.01% was observed for an applied electric field of 3 V/micron for a 100 nm thick film. The Kerr coefficient as determined is about 1.7x10^{-11} m/V^2. This exceptionally large quadratic electro-optic effect has been attributed to the confinement of this charge-transfer system within a sub-nanometer dimension. A. Narayanan, A. Palthi and M. Thakur, J. Macromol. Sci. – PAC, accepted.

9:48AM H20.00008 Quadratic Electro-optic Measurements in Nonconjugated Conductive Polymers, iodine-doped Polyisopropene and Poly(β-pinenes) at 1.55µm, ANANTHAKRISHNAN NARAYANAN, JITTO TITUS, MRINAL THKUR, Photonic Materials Research Laboratory, Auburn University, AL. — Exceptionally large near-resonant (at 633nm) quadratic electro-optic effects in nonconjugated conductive polymers, iodine-doped poly(β-pinenes) and 1,4-cis-polyisopropene have been previously reported. In this report, we discuss the quadratic electro-optic effects in these polymers at 1.55µm. The measurements were made using the field-induced birefringence technique. A modulation depth of about 0.1% was observed for a 1 µm thick sample of doped poly(β-pinenes) at an applied field of 1V/µm. The Kerr coefficient as determined was about 1.6x10^{-10} m/V^2. For polyisopropene the modulation was slightly smaller. These exceptionally large Kerr coefficients at a technologically important wavelength make these polymers promising for guided-wave applications in electro-optics. Techniques for longer-term stability of the samples have been established. The large optical nonlinearities as observed have been attributed to the sub-nanometer confinement of these charge-transfer systems.

10:00AM H20.00009 ABSTRACT WITHDRAWN —

10:12AM H20.00010 Ultrasensitive Solution Processed Polymer Photodetectors. XIONG GONG, MING-HONG TONG, GANG YU, CHAN-LONG SHIEH, BOO NILSSON, ALAN HEEGER, CBRITE INC TEAM, UC SANTA BARBARA TEAM. — Semiconducting polymeric optoelectronic and electronic devices have evolved as a promising cost-effective alternative to silicon-based devices. Organic photodetectors have been the subject due to several inherent advantages. Some of the important advantages of these so-called “plastic” electronics include large-area detection, low cost of fabrication, ease of processing and mechanical flexibility. However, there are few reports on organic photodetectors whose performances are comparable with inorganic counterparts. We report ultrasensitive solution processed photodetectors fabricated by different semiconducting polymers as the electron donors and various fullerences derivatives and/or inorganic quantum dots as the electron acceptors. Polymer photodetectors with different photo-responsivity and detectivity were demonstrated. One example is that polymer photodetectors have photo-response from 300nm to 1450nm, the detectivity larger than 10^{12} cm Hz^{1/2}/W, and linear dynamic range larger than 120 dB. All these values are comparable to or even better than their inorganic counterparts.

10:24AM H20.00011 Twin instability of Peierls distortion and its mechanical consequence on conductive polymer actuation, MINGHAI LI, ANDRE BOTELOHO, XI LIN, Boston University. — We prove analytically that a one-dimensional metallic chain is subject to two coupled spontaneous conformational relaxations, resulting in the well-known Peierls bond length alternation and an overall chain contraction. Using the Su-Schrieffer-Heeger (SSH) Hamiltonian, a tight-binding version of the Peierls theory, we find in a neutral defect-free polyacetylene chain these two coupled distortions work cooperatively against the backbone elastic deformation. The cooperative bond alternation and chain contraction deformations have two effects, allowing bonds alternate and contract less than the case when deformations are independent and breaking the charge conjugation symmetry which would otherwise be conserved. Making such a deformed neutral chain as the reference, we find that creation of self-localized solitons upon dopings results in spontaneous chain contractions within the self-localized domains where the anti-Peierls distortions are enforced. Our numeric results based on the SSH model and first-principles calculations indicate that chain contractions are proportional to the soliton density at low dopings, and the overall chain length varies non-monotonically with respect to the doping level, reaching a maximum contraction of 0.15% at 5% doping.

10:36AM H20.00012 Soliton migration along trans-polyacetylene backbone, MINGHAI LI, YONGWOO SHIN, XI LIN, Boston University. — We compute the minimum energy paths and activation barriers for the soliton migration process along trans-polyacetylene backbone via the Su-Schrieffer-Heeger (SSH) model and ab initio calculations. Our results confirm the conventional consensus that soliton hops over two CH sites in one single step, maintaining wavefunction nodal structures at intermediate CH sites. Standard SSH parameters give rise to negligible migration barriers, which increases exponentially as the localization width decreases. Favoring the opposite elastic strain as the boundaries, soliton prefers staying at the center of an open chain; this ground state energy increases linearly when the chain length decreases. Starting at the center and moving towards the chain termination, soliton first sees a quadratic wash-board energy landscape when it is far away from the boundary and then smoothly switches to an exponentially increased wash-board energy landscape when it is in the vicinity of the boundary due to its localization width shrinkage. The local minima energy has a larger exponent compared to that of the activation barrier so they cross each other at a certain point, beyond which the barrier disappears and solitons cannot get closer to the boundary.

10:48AM H20.00013 ABSTRACT WITHDRAWN —

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H21 FIAP: Spectroscopic Studies of Semiconductors 323

8:00AM H21.00001 Two- and three-photon absorption of germanium in the mid-infrared, DONGMIN SEO, LEONARD FELDMAN, NORMAN TOLK, PHILIP COHEN. — We have studied the nonlinear optical response of crystalline germanium using high-power infrared picosecond laser pulses at wavelengths ranging from 2.8 µm to 5.2 µm. Transmittance as a function of fluence at 2.8 µm and 4.4 µm were fitted by using two- and three-photon absorption, respectively. Data at 3.2, 3.6, and 4.0 µm, however, required consideration of simultaneous two- and three-photon absorptions in order to fit the experimental data. Transmittance as a function of wavelength further supports the onset of the two- and three-photon absorption at appropriate wavelengths.

3Honda R&D

The National Science Foundation supported this research. The W. M. Keck Foundation Free electron laser at Vanderbilt University is acknowledged.
Owing to the bi-stable nature of the Si donor, samples cooled in the dark are insulating. In the present work, an infrared LED is used to photodope 0 OHNO, Tohoku University — Highly Si-doped Al persistent photoconductivity, JENNIFER MISURACA, STEPHAN VON MOLNAR, PENG XIONG, MARTECH, Florida State University, 0 be extracted for various illumination times as the Fermi energy is tuned systematically. Application to Si-doped Al Soc. Jpn. 56, 2259 (1987) [2] I. Terry, et al. Solid State Commun. 84, 235 (1992)

For Ns higher than 6 10 11, only this new interaction is clearly visible though its amplitude decreases when increasing Ns. The origin of this new interaction is very likely related to mechanisms involving phonons. The different possibilities are discussed.

We study ensembles of phosphorus donor bound excitons in Si via photocurrent measurements at low temperatures since Auger non-radiative decay process is primarily dominant in an indirect band-gap semiconductor such as Si. We report electric and magnetic field effects on photocurrent signals of phosphorus donor bound excitons.

1also at University of Tokyo, Japan
2also at National Institute of Informatics, Japan
3also at National Institute of Informatics, Japan

4:00AM H21.00007 Determining the bandtail shape of highly Si-doped Al 0.3 Ga 0.7 As using persistent photoconductivity, JENNIFER MISURACA, STEPHAN VON MOLNAR, PENG XIONG, MARTECH, Florida State University, JELENA TRBOVIC, Institute of Physics, University of Basel, JUN LU, JIANHUA ZHAO, Institute of Semiconductors, Chinese Academy of Sciences, HIDEO OHNO, Tohoku University — Highly Si-doped Al 0.3 Ga 0.7 As can be driven through the metal-insulator phase transition using persistent photoconductivity [1]. Owing to the b-stable nature of the Si donor, samples cooled in the dark are insulating. In the present work, an infrared LED is used to photodope the sample at SK for a range of illumination times, which populates shallow states and provides a way to change the carrier concentration of the sample in situ. Measuring the carrier concentration as a function of temperature allows for the finite temperature carrier concentrations and Hall activation energies to be extracted for various illumination times as the Fermi energy is tuned systematically. Application to Si-doped Al 0.3 Ga 0.7 As prepared by MBE allows one to infer the bandtail shape in the energy range between the Fermi energy of the unilluminated sample and the mobility edge. [1] S. Katsumoto, et al. J. Phys. Soc. Jpn. 56, 2259 (1987) [2] I. Terry, et al. Solid State Commun. 84, 235 (1992)
9:24AM H21.00088 Effect of order/disorder near the Γ-L and L-X crossovers in the conduction band of lattice-mismatched Ga$_x$In$_{1-x}$P alloys\textsuperscript{1}, L. BHUSAL, M. STEIJNER, J. GEISS, A. MASCARENHAS, National Renewable Energy Laboratory, 1617 Cole Blvd, Golden CO-80401 — In this work we studied the effect of order/disorder on the Γ-L and L-X crossover points in the conduction band of Ga$_x$In$_{1-x}$P alloys, using polarized photoluminescence and electroreflectance techniques at various temperatures. Ga$_{x}$In$_{1-x}$P samples ($x$=0.25-0.78) were grown by atmospheric pressure organometallic vapor phase epitaxy (OMVPE). Some samples were grown directly on a miscut GaAs substrate while in other samples a thick GaAsP step grade was grown first, to reduce the dislocation density. The significance of the crossover point in the conduction band of the alloy for the efficiency of devices such as multijunction high-efficiency solar cells and light emitting diodes will be discussed.

9:36AM H21.00009 Intersubband absorption in InAlN/GaN heterostructures, O. MALIS, C. EDMUNDS, Binghamton University, Binghamton, NY, M. J. MANFRA, D. L. SIVCO, Bell Labs, Alcatel-Lucent, Murray Hill, NJ, R. MOLNAR, MIT Lincoln Laboratories, Lexington, MA — Nitride superlattices are promising for intersubband light emission and detection in the currently inaccessible near-infrared range (2-3 µm). Efforts to explore the intersubband properties of nitrides have been hampered so far by difficulties related to the quality of the materials. Most studies to date have employed AlGaN/GaN heterostructures. However, the large lattice mismatch between AlGaN and GaN limits the total thickness of the structures. We are focusing on lattice-matched InAlN/GaN superlattices. InAlN has been less investigated due to the challenges in growing high-quality In-containing nitrides. Nevertheless, the large conduction band offset (1 eV) and lack of piezoelectric effect make the lattice matched nitrides ideally suited for near-infrared applications. We have performed a detailed intersubband absorption study of InAlN/GaN superlattices grown by MBE on HVPE GaN templates. X-ray diffraction analysis suggests that our samples are among the highest quality ever reported. The band structure of the materials was examined with Fourier-transform infrared spectroscopy. Strong intersubband absorption in the 430-530 meV energy range is reported for the first time for 2-4.5 nm-wide quantum wells.

9:48AM H21.00010 Beryllium acceptor binding energy in AlN. ASHK SEDHAIN, T. M. AL TAHTAMOUNI, JING LI, Kansas State University, JINGYU LIN, HONGXING JIANG, Texas Tech University, DEPARTMENT OF PHYSICS, KANSAS STATE UNIVERSITY COLLABORATION, NANO-TECH CENTER AND DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, TEXAS TECH UNIVERSITY COLLABORATION — The acceptor binding energy of an alternate dopant, Be, in AlN epi-layers has been probed by time-resolved photoluminescence (PL) spectroscopy. The binding energy of excitons bound to Be acceptors in AlN is determined to be about 33 meV, which implies that the Be acceptor binding energy in AlN is about 0.33 eV in accordance with Haynes’ rule. The measured PL decay lifetimes of the acceptor-bound exciton transitions in Be- and Mg-doped AlN (95 and 119 ps, respectively) also indicate that the binding energy of Be is smaller than that of the most common acceptor dopant in AlN, namely, Mg. The smaller activation energy of Be in AlN has the potential to partly address the critical p-type doping, issue in AlN- and Al-rich AlGaN by increasing the room temperature free hole concentration by ~10$^3$ compared to the case of Mg doping.

10:00AM H21.00011 Estimation of third-order nonlinear optical susceptibility $\chi^{(3)}$ of synthetic Cu$_2$O crystal\textsuperscript{1}, SHAHIN MANI, JOON JANG, JOHN KETTERSON, Department of Physics & Astronomy, Northwestern University, KETTERSON’S TEAM — High-quality crystals of Cu$_2$O were prepared by an improved method for thermally oxidizing metallic copper. We report the nonlinear refractive index $n_2$ and the nonlinear absorptive index of the Cu$_2$O crystals. The following methods were utilized: (i) Z-scan, (ii) third-harmonic generation, and (iii) intensity-dependent interferometry. The third-order susceptibility $\chi^{(3)}$ of a material plays an important role in optical signal processing including switching, altering the frequency and the transmission characteristics. A comparison between the third-order nonlinear susceptibilities of a standard nonlinear reference material, carbon disulfide (CS$_2$) and Cu$_2$O will be made.

1 Supported by the National Science Foundation under grant CCF 03-29957.

10:12AM H21.00012 Anomalous Fresnel coefficients for quadrupole polaritons in Cu$_2$O\textsuperscript{1}, JOON JANG, YI SUN, SHAHIN MANI, JOHN KETTERSON, Department of Physics, Northwestern University, KETTERSON’S TEAM — In a direct-gap semiconductor, a polariton is a quantum superposition of an excitation and a photon, formed near the light cone. Unlike dipole polaritons, a quadrupole polariton in a bulk Cu$_2$O is a coherently propagating bosonic state with an unusually long decoherence time owing to its unusual underlying electronic structure. Therefore, this unique semiconductor provides a model system for studying the theory of so-called additional boundary conditions at the vacuum-crystal boundary. Using resonant two-photon excitation, we create a coherently propagating polariton wave packet at 2 K and measure its reflectance (R) and transmittance (T) at the boundary opposite to the incoming surface. Surprisingly, we find an enhanced reflection of polaritons from sample surfaces such that the ratio R/T deviates significantly from the present theory. This anomalous boundary effect most likely arises from the quadrupole excitonic (matter) component of polaritons. Our experimental results have implications for the design of polariton-based waveguides and resonators in which traveling polaritons are effectively confined in the medium.

1 Supported by the NSF under grant CCF 03-29957.

10:24AM H21.00013 Photoluminescence Characteristics of Pulsed Laser Deposited ZnO Thin Films Grown in Nitrogen/Oxygen Ambients, M.A. THOMAS, J.B. CUI, Y.C. SOO, H. KANDEL, T.P. CHEN, University of Arkansas-Little Rock, C.P. DAGHLIAN, Dartmouth College — ZnO thin films were grown by pulsed laser deposition using a Zn target in different atmospheres. The samples were characterized by X-ray diffraction, energy dispersive X-ray analysis and temperature dependent photoluminescence (PL) measurements. The growth conditions were varied sequentially from a pure oxygen to a pure nitrogen atmosphere. The band structure of the materials was examined with Fourier-transform infrared spectroscopy.

10:36AM H21.00014 Optical properties of epitaxial ZnGeAs$_2$ thin film, S.G. CHOI, NREL, D.E. ASPNES, NCSU, M. VAN SCHILFGAARDE, ASU, T.J. PESHEK, T.J. COUTTS, A.G. NORMAN, J.M. OLSON, D.H. LEVI, NREL — Chalcopyrite ZnGeAs$_2$ lattice-matched to GaAs(001) is a promising 1.1 eV band gap semiconductor for applications in non-linear photonic devices and multijunction solar cells. Knowledge of the optical properties of epitaxial ZnGeAs$_2$ is essential for device applications. We present room temperature optical properties of a ZnGeAs$_2$ thin film grown epitaxially on a GaAs(001) substrate by metalorganic vapor phase epitaxy. Spec troscopic ellipsometry was employed to measure the pseudoelectric function of the ZnGeAs$_2$ thin film, and was compared with a theoretical calculation within the quasiparticle self-consistent GW approximation. The interband-transition critical-point energies were obtained from a standard lineshape analysis of the measured spectrum. We will also present a comparison of the optical properties of ZnGeAs$_2$ with those of other II-IV-V$_2$ chalcopyrite compounds as well as their corresponding III-V zincblende compounds. This abstract is subject to government rights.
In particular, Mn ions doped into GaAs quantum wells have spin lifetimes close to several nanoseconds and can be optically manipulated in zero magnetic field. In contrast, in bulk GaAs and semiconductors, the spin relaxation rate is much faster due to phonon scattering. To study this system in the low density limit, we incorporate a distributed Bragg reflector optical cavity around the Mn containing wells, which enhances Mn luminescence and allows spatial isolation of a small number of Mn ions imaged using scanning microphotoluminescence. In such structures, we observe unusually long Mn spin lifetimes.

To study this system in the low density limit, we incorporate a distributed Bragg reflector optical cavity around the Mn containing wells, which enhances Mn luminescence and allows spatial isolation of a small number of Mn ions imaged using scanning microphotoluminescence. In such structures, we observe unusually long Mn spin lifetimes. We discuss the effect of cavity coupling on spin dynamics Mn ions in the single ion limit.

This work was supported by the AFOSR, NSF, and ONR.


This work was supported by AFOSR and ARO.

M. Yasar, A. Petroiu, S. Suny at Buffalo, Buffalo NY, C. Li, A. Hanbicki, G. Kioseoglou, B. Jonker, Naval Research Laboratory, Washington D.C. — We have carried out optical pumping, Hanle and longitudinal Hanle studies of InGaAs:Al/GaAs quantum wells. The circular polarization at zero magnetic field has a maximum around 50 K indicating that at low temperatures the recombination is associated with a bound electron. The measured spin lifetimes at low temperatures are an order of magnitude longer than those measured in reference GaAs/AlGaAs quantum wells. This is attributed to the suppression of the Dyakonov-Perel spin relaxation mechanism in this bound system. As the temperature is increased from 5 to 50 K the spin lifetimes decrease and become comparable to the lifetimes of the reference sample. In the longitudinal Hanle geometry the circular polarization increases with magnetic field and reaches a maximum at B = 1.5 tesla. Beyond 1.5 tesla the circular polarization decreases. A series of polarization oscillations superimposed on the decreasing background with a periodicity of approximately 1 tesla is observed. These oscillations are tentatively attributed to the variations in the magnetic flux through the bound electron orbit. Work at SUNY was supported by ONR and NSF.
9:36AM H22.00007 Spontaneous Loss of Spin Coherence in GaAs/Si Heterostructure

GUANGLEI CHENG, PATRICK IRVIN, Department of Physics and Astronomy, University of Pittsburgh, BQIN HUANG, IAN APPELBAUM, Department of Physics, University of Maryland, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh — We present a possible way to optically inject spins into silicon. In this work, GaAs and Silicon-on-Insulator (SOI) wafers are bonded together by an ultrathin Ag layer using UHV wafer bonding. Standard optical pump-probe Kerr microscopy technique is applied to examine the spin coherence in the GaAs/Si heterostructure. In some areas of the bonded wafer, a relatively long spin coherence time of T2*=0.5 ns is observed in the GaAs. In other parts of the sample, the spin coherence is observed to decay much more rapidly (T2*=140ps). One possible explanation is that the quality of the bond varies across the wafer and that the strongly bonded areas exhibit spin transport from GaAs to silicon.

1 This work is supported by NSF Materials World Network DMR-0602846.

9:48AM H22.00008 Coherent optical control of correlation waves of spins in semiconductors

ERAN GINOSSAR, Yale University, YEHOUSA LEVINSON, SHIMON LEVIT, Weizmann Institute of Science — We calculate the dynamical fluctuation spectrum of electronic spins in a semiconductor under a steady-state illumination by light containing polarization squeezing correlations. Taking into account quasi-particle lifetime and spin relaxation for this non-equilibrium situation we consider up to fourth order optical effects which are sensitive to the squeezing phases. We demonstrate the possibility to control the spin fluctuations by optically modulating these phases as a function of frequency, leading to a non-Lorentzian spectrum which is very different from the thermal equilibrium fluctuations in n-doped semiconductors. Specifically, in the time-domain spin-correlation can exhibit time delays and sign flips originating from the phase modulations and correlations of polarizations, respectively. For higher light intensity we expect a regime where the squeezing correlations will dominate the spectrum.

1 Deceased.

10:00AM H22.00009 Time Resolved Spectroscopy of InSb Quantum Wells Using Differential Transmission Technique

K. NONTAPOT, M. BHOWMICK, G.A. KHODAPARAST, Virginia Tech., S.J. CHUNG, M.B. SANTOS, University of Oklahoma — The growing interest in spin-related phenomena and devices has prompted intense activity in the science and engineering of narrow gap semiconductors (NGS). NGS offer several scientifically unique features such as small effective masses, large g-factors, high intrinsic mobilities, and large spin-orbit coupling effects. In this work we report the dynamics of photo-excited carrier/spin in several InSb/AlxIn1−xSb based quantum wells (QWs) using differential transmission spectroscopy. The InSb QW layers were selectively pumped and probed by mid-infrared pulses to avoid possible contributions from the barrier materials. We compare our results with the earlier measurements using magneto-optical Kerr (MOKE) effect. Our results are important to understand different relaxation mechanisms in NGS with strong-spin orbit interactions.

1 Supported by: NSF-DMR-0507866, NSF-DMR-0520550.

10:12AM H22.00010 Spin polarized current in InSb based structures

M. FRAZIER, M. BHOWMICK, J.J. HEREMANS, G.A. KHODAPARAST, Virginia Tech., S.J. CHUNG, M.B. SANTOS, University of Oklahoma, X. LIU, J. FURDYNA, University of NotreDame — Recently, there has been much interest in developing and exploring spin based semiconductor devices and phenomena. One of the key challenges in developing spin based devices is to generate, control, and measure spin currents directly. In this talk, we report interband circular photogalvanic (CPG) effects using pulsed near-infrared radiation in InSb quantum wells and two InSb films grown on GaAs and InP substrates. We observe a CPG current whose direction and magnitude depend on the helicity of the incident light, the angle of incidence, and temperature. Our observation is important to understand zero-field spin splitting mechanisms in a system with strong spin-orbit interaction.

1 Supported by: NSF-DMR-0507866, NSF-DMR-0603752, NSF-DMR-0520550, NSF-DMR-0618235, AFOSR Young Investigator Program 06NE231.

10:24AM H22.00011 Optically-Induced 13C Nuclear Spin Polarization through Nitrogen-Vacancy Centers in Diamond

JONATHAN KING, PATRICK COLES, JEFFREY REIMER, University of California-Berkeley — The spin-1 negatively charged nitrogen-vacancy (NV) center in diamond has received much attention for its long spin-coherence times and optical polarization into the m_s=0 sublevel. These properties make it attractive for applications such as quantum information processing and high-resolution magnetometry. Large nuclear polarizations in diamond may be useful to quench decoherence, as an initialization step for quantum computing, or as a platform for enhancement of nuclear magnetic resonance (NMR) signal in dilute spin systems. In this work, we demonstrate the polarization of the bulk 13C nuclear spin system by interaction with the optically polarized NV center system at 9.4 Tesla and 5K nominal temperature. Large nuclear polarizations are observed through Faradic detection of bulk 13C NMR signals. The signals are opposite in sign to thermally-generated signals, indicating nuclear polarization into the m_f = -1/2 sublevel. We model the phenomenon and propose microscopic mechanism for the polarization.

1 Supported by NSF under project ECS-0608763.

10:36AM H22.00012 Optical hyperpolarization of the nuclear and electronic spins of 31P in 28Si

A. YANG, M. STEGER, T. SEKIUCHI, M. M. W. THEWALT, Dept. of Physics, Simon Fraser University, Burnaby, BC, Canada, T. D. LADD, E. L. Ginnot Laboratory, Stanford University, Stanford, CA, USA, K. M. ITOH, Keio University and CREST-JST, Yokohama, Japan, H. Riemann, N. V. Abrosimov, Institute for Crystal Growth (IKZ), Berlin, Germany, P. Becker, PTB Braunschweig, Braunschweig, Germany, H.-J. Poehl, VITCON Projectconsult GmbH, Jena, Germany, J. W. Ager III, E. E. Haller, UC Berkeley and LBNL, Berkeley, CA, USA — We have recently shown that the donor hyperfine splitting can be resolved for the 31P donor bound exciton in highly enriched 28Si, enabling either optical or optical-electrical readout of the electronic and nuclear spin state of this promising qubit candidate.[1] Here we show that these same optical transitions can be used to quickly achieve large nuclear and electronic hyperpolarizations of the 31P donor in 28Si. This may provide a viable solution to the problem of initializing the nuclear spins, a roadblock for quantum computing schemes involving nuclear spins in Si. We also report on the remarkably narrow homogeneous linewidth of this bound exciton transition, measured by hole burning spectroscopy. This suggests that even higher spin selectivity and hyperpolarization may be achievable in more highly enriched 28Si, or when dealing with individual 31P donors. [1] A. Yang et al., Phys. Rev. Lett. 97, 227401 (2006).
10:48AM H22.00013 Time-resolved Infrared Magnetospectroscopy of GaAs at the NSLS
G.L. CARR, NSLS, Brookhaven National Lab, J.J. TU, Physics Department, City College of the City Univ. of NY — We describe a facility for performing photoinduced time-resolved infrared spectroscopy of materials in magnetic fields up to 10T at beamline U4IR of the National Synchrotron Light Source (NSLS). The facility combines an existing time-resolved capability (based on pulsed synchrotron radiation and a synchronized Ti:sapphire laser to achieve ~100 ps resolution) with a split-coil superconducting solenoid and optical cryostat. We also report a THz study of photocarrier and exciton dynamics in GaAs using this facility. It is found that, for B>0, a portion of the photo-induced carrier absorption appears as an electron cyclotron resonance, while the exciton unbinding absorption splits into spin and orbital transitions (Zeeman effect). At low temperatures, we observe that the relaxation of photocarriers toward the band edge involves the breaking of existing excitons, leading to a combination of absorption and bleaching features that evolve on a ~1 ns time scale.

1Supported by DOE under contract DE-AC02-98CH10886 at the NSLS of Brookhaven Natl Lab. Portions of the time-resolved program supported under DE-FG02-02ER45984 at Univ. of Florida.

Tuesday, March 17, 2009 8:00AM - 10:48AM –
Session H23 FIAP DCMP: Optical and Spectroscopic Properties and Nano 325

8:00AM H23.00001 Photoemission core level shifts and phonon broadening for Cs film on Cu(100)
XUBING ZHOU, KEVIN KOCH, J.L. ERSKINE — Department of Physics, University of Texas at Austin, Austin, TX 78712. We have measured Cs 5p photoemission core level broadening data for Cs film on Cu(100) at different temperatures and have obtained bulk-atom and surface-atom values of the zero-temperature phonon width and the effective Debye temperature, which governs the temperature dependence of the broadening. The coupling constant C for alkali metals in the phonon-broadening theory of Hedin and Rosengren[1] is about 30% higher in the surface than in the bulk. This result is compared with experiment results on other alkali metals[2]. We also studied the temperature dependent binding energy shifts for the Cs 5p core level peaks and our data fit the lattice expansion theory very well except at temperature higher than 220 K. At high temperature deviations are proved to be caused by thermal evaporation of Cs film. [1] L. Hedin and A. Rosengren, J. Phys. F. 7, 1339 (1977). [2] D.M. Riffe and G.K. Wertheim, Phys. Rev. B 61, 2302 (2000).

8:12AM H23.00002 Auger-Photoelectron Coincidence Spectroscopy measurement of the secondary electron distribution from 0 eV to 81 eV, created by the MVV Auger transition in Cu (100) , K. SHASTRY, S. MUKHERJEE, A.H. WEISS, University of Texas at Arlington, S.L. HULBERT, Brookhaven National Laboratory, R.A. BARTYN-SKI, Rutgers University — In conventional spectroscopic measurements, low energy Auger lines are superimposed upon a large background due to secondary electrons that arise from loss processes that are unrelated to the Auger process. Here we present the results of measurements in which Auger-Photoelectron coincidence techniques were used to eliminate background unrelated to the Auger process and obtain the energy distribution of electrons emitted as a result of the M_{2,3}VV transition in Cu (100) over the full range of emitted energies (0 eV – 81 eV). The measurements revealed a well formed Auger peak at ~60eV accompanied by a low energy tail (LET) associated with the MVV transition. The LET extends to 0 eV and has a broad maximum at ~ 7eV. The integrated intensity of the LET was ~ 6 times larger than that of the Auger peak itself. The origin of the LET will be discussed in terms of extrinsic mechanisms in which electrons from the peak lose energy as they propagate to the sample surface, as well as intrinsic mechanisms in which multi-electron Auger processes distribute the energy gained by the filling of the core-hole to multiple electrons.

8:24AM H23.00003 Ultrafast Spectroscopy on Solids at FLASH
DAVID BERNSTEIN, Stanford University, YVES ACREMANN, ANDREAS SCHEHRZ, SLAC, MARTIN BEYE, ALEXANDER FÖHLISCH, WILLIAM SCHLOTTER, DESY, TORBIN BEECK, FLORIAN SORGENFREI, ANNETTE PIETZSCH, WILFRIED WURTH, DESY, JOACHIM STÖHR, SLAC — X-ray/VUV free electron laser (FEL) facilities such as FLASH, LCLS, and the European X-FEL open the door to a wide variety of exciting experiments in x-ray physics. Due to the rapidly stochastic processes governing FEL radiation and the difficulties in tuning an FEL, it has not been clear whether spectroscopy could be done using such sources. Here we demonstrate the feasibility of doing near edge x-ray absorption fine structure (NEXAFS) spectroscopy on solids. Samples consisting of LaMnO and Al films, respectively, were lithographically fabricated on thin silicon nitride membranes. Ultrafast femtosecond pulses of radiation from the FLASH FEL were dispersed by the monochromator grating at beamline PG2 and impinged upon the samples. Absorption was measured in transmission using a Ce:YAG crystal and imaged by an intensified CCD. The incident intensity was measured through a blank nitride membrane next to the sample. We discuss the possibility of both subsurface Ce and Te as giving rise to this signal; density functional theory calculations indicate that the subsurface Ce atom gives a more significant contribution to the overall tunneling current.

8:36AM H23.00004 STM study of CeTe2: contribution of the subsurface lattice
ALEKSANDRA TOMIC, JOSH VEAZEY, ZSOLT RAK, CHRISTOS MALLIKAKAS, MERCOURI KANATZIDIS, S. D. MAHANTI, STUART TESSMER — We have studied the nature of the surface charge distribution in CeTe2 with scanning tunneling microscopy (STM). At 77 K, the STM topography and Fourier transform show both the atomic lattice of surface Te atoms arranged in a square net and the CDW modulations oriented at 45 degrees with respect to the Te net. In addition, we observe peaks in the Fourier transform that we attribute to atoms lying below the surface Te net. We discuss the possibility of both subsurface Ce and Te as giving rise to this signal; density functional theory calculations indicate that the subsurface Ce atom gives a more significant contribution to the overall tunneling current.

8:48AM H23.00005 Effect of a Fe substitutional impurity on the geometric and electronic structure of Au13 cluster
GHAZAL SHAFAI, TALAT RAHMAN, University of Central Florida — We have carried out spin-polarized density functional theory calculations based on the potential method to determine the changes in the characteristics of the Au13 cluster when one Au atom is replaced by Fe. For a pure Au13 cluster, the 2D geometry is the lowest-energy isomer, followed closely by a flake structure, while the icosaedron is higher in energy by ~2.98 eV and is not stable since it is found to undergo Mackay transition to form a cuboctahedron. When a surface or central Au atom is replaced by Fe, we find dramatic changes in the energy ordering of these nanoparticles, since Fe tries to move inwards so as to be highly coordinated. In fact the distorted icosaedron and a biplanar structure obtain the lowest energy. The structure of the Fe-centered icosaedron is slightly distorted (Jahn-Teller distortion), so that the degeneracy on two bands near Fermi level is removed. The lowest energy isomer in this study has the highest magnetic moment (3.98 μB) in comparison with that of the other isomers. The magnetic moment of the icosaedron with an Fe atom at the center is 3.1 μB, which is in agreement with previous findings.

1Work supported in part by DOE, under grant number DE-FG02-02ER45634

9:00AM H23.00006 ABSTRACT WITHDRAWN —
9:12AM H23.00007 Size-dependent crystallinity of nano-Pt/$\gamma_2\text{Al}_2\text{O}_3$1. LONG LI, Eng and Materials Sci Dept, Univ of Pittsburgh, L.-L. WANG, S. I. SANCHEZ, J. H. KANG, Univ of Illinois, Q. WANG, Yeshiva Univ, Z. ZHANG, Univ of Pittsburgh, A. I. FRENKEL, Yeshiva Univ, R. G. NUZZO, D. D. JOHNSON, Univ of Illinois, J. C. YANG, Univ of Pittsburgh — Metallic platinum nanoparticles (NP) on $\gamma_2\text{Al}_2\text{O}_3$ powders were synthesized with a size range from sub- to several nanometers. High-resolution transmission electron microscopy (HRTEM) studies revealed a size-dependent crystallinity of the Pt NPs, where Pt NPs with size $<1$ nm had a disordered structure, Pt NPs with size $>2.5$ nm all showed a crystalline structure. For Pt NPs with sizes between 1.1 and 2.4 nm, a transition zone exists in which $\sim85$% of NPs appeared disordered and $\sim15$% ordered. X-ray absorption spectroscopy (XAS) measurements support this result where increasing-disorder distribution of Pt-Pt bond lengths was noted with decreasing Pt nanoparticle size. A search for ground state structure of Pt$_{\gamma_2}/\gamma_2\text{Al}_2\text{O}_3$ (100) with density functional theory (DFT) showed that the disordered structure is energetically more favorable than the ordered close-packed structures by 1.53 eV at the size of 1.1 nm.

1DOE-BES funding, DE-FG02-03ER15476

9:24AM H23.00008 Size Distribution of Nano-Crystallites in Non-Crystalline Binary Alloys, YONG W. KIM, Lehigh University, ANDREW ABRAHAM, Moravian College, JERRY KIM, UCLA — The factors that affect thermophysical property determination for non-crystalline metallic alloys include non-uniformities in compositional and morphological property within a specimen. A series of measurements have shown that a specimen’s thermal history leads to a spatial profile of elemental composition that differ from one specimen to another for the same alloy. (See Y.W. Kim, Int. J. Thermophysics 28, 732 (2007), and references therein.) In order to develop a theoretical model for temperature dependence of thermophysical properties, we consider thermal dissociation of nano-crystallites within a randomly close-packed (RCP) medium. Once the size distribution of the nano-crystallites has been established at a given temperature, a set of coupled dissociation equations can be solved at all other temperatures. Transport properties can then be computed over a range of temperature. In this paper we present the size distribution of crystallites in a bed of RCP spheres. Two different size spheres are mixed at several compositions to simulate non-crystalline binary alloys in 2-D. The distribution is found to be peaked at a crystallite size specific to a given alloy composition. This work is support in part by the NSF-DMR(Metals).

9:36AM H23.00009 Irreversibility in Cooling and Heating Processes in the Magnetocalic MnAs and Alloys1, A.L. LIMA SHARMA, Dept. Physics, Tuskegee University, Tuskegee, AL 36088, S. GAMMA, Dept. of Physics, Univ. Fed. do Est. de Sao Paulo, Rua Prof. Artur Riedel, 275 - Jd. Eldorado - Diadema- SP 00972-270 - Brazil, A.A. COELHO, Inst. de Física Gleb Wataghin, Univ. Est. de Campinas (UNICAMP), C. P. 6165, Campinas, SP 13083-970 - Brazil — Irreversibility of adiabatic processes in the magnetocaloric MnAs and alloys are presented here. We used a differential scanning calorimeter in order to record the heat flux as a function of the temperature and applied field for MnAs, Mn$_0$$_1$$_9$$\gamma$$_2$$F$_0$$0$$_0$$0$$_0$$_0$ As and Mn$_0$$_1$$_9$$\gamma$$_2$$A$_0$$0$$_0$$0$$_0$As. From the measured heat flux, we extracted the latent heat and entropy associated to cooling and heating processes. In the cooling curve, we observed that $S_{c}$$\gamma$$_2$$F$_0$$0$$_0$$0$$_0$$ > S$_{c}$$\gamma$$_2$$A$_0$$0$$_0$$0$$_0$$ > S$_{c}$$\gamma$$_2$Mn$_0$$_1$$_9$$_0$$_0$$_0$$_0$$_0$ As, the index $c$ refers to cooling process, similarly, for the heating process: $S_{h}$$\gamma$$_2$$F$_0$$0$$_0$$0$$_0$$ > S$_{h}$$\gamma$$_2$$A$_0$$0$$_0$$0$$_0$$ > S$_{h}$$\gamma$$_2$Mn$_0$$_1$$_9$$_0$$_0$$_0$$_0$$_0$$_0$$_0$ As. On the doped samples, the thermomagnetic behavior is compatible with a scenario where Zener’s $p$- $d$ exchange mechanism dominates, i.e. the interaction range is weaker but long ranged, because the extended valence hole states mediate the ferromagnetic interaction. The difference of the entropy obtained from cooling and heating process was found to be as high as 37%.

1to appear in Applied Physics Letters

9:48AM H23.00010 Semiconductor behavior in bcc Cr$_{1-x}$Al$_x$ thin films1, Z. BOEKELHEIDE, F. HELLMAN, University of California, Berkeley — Cr$_{1-x}$Al$_x$, with $x=0.15$-$0.25$, has semiconducting electronic properties: extremely high resistivity and a negative temperature coefficient of resistance, along with a gap in the infrared reflectivity. This is unusual for an alloy of two metals, but similar behavior has been observed in Fe$_3$VAl and has been attributed to a hybridization-induced band gap. In bulk, Cr$_{1-x}$Al$_x$ is known to be inhomogeneous, with two crystal phases coexisting: one, a disordered bcc solid solution, and the other, called the “X-phase”, with a microstructure consisting of 1-3nm domains. Because of this inhomogeneity, it was previously not known which phase was responsible for the semiconductor behavior. We used epitaxial thin film growth techniques to preferentially nucleate the bcc phase and study the effect of crystal structure on the electronic properties. We found that films grown epitaxially on MgO (100) substrates, expected to grow preferentially in the bcc phase, have high resistivity like bulk Cr$_{1-x}$Al$_x$ while polycrystalline films grown on amorphous SiO$_2$ have lower resistivity. This suggests that the semiconductor behavior is intrinsic to the bcc structure.

1This work was supported by the Director of the Materials Sciences and Engineering Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

10:00AM H23.00011 Exciton Recombination in Nanometer-Wide GaN/AlN Quantum Wells. ZHENWEN PAN, MADALINA FURIS, University of Vermont, Burlington, VT, ALEXANDER N. CARTWRIGHT, University at Buffalo - SUNY, Buffalo, NY, WILLIAM J. SCHAFF, Cornell University, Ithaca, NY — In nitride semiconductor heterostructures, the presence of very strong built-in electric fields, oriented perpendicular to the semiconductor layers, dramatically impacts the electronic states, excitonic recombination, and photoluminescence in these materials. The origins of these fields lie in the non-centro- symmetric character and the strong piezoelectricity of the heterostructures. We investigated electronic states in the presence of strong built-in fields ($\sim$5 MV/cm) in very narrow, nanometer-wide GaN/AlN quantum wells via time-resolved photoluminescence spectroscopy. We find that the strong confinement ($\sim$2eV in the conduction band) leads to significant overlap in the electron and hole wavefunctions, even in the presence of large built-in fields. The temperature dependence of radiative lifetimes and emission energies indicates the band-edge recombination contributions (i.e., excitonic and/or shallow -acceptor pair) dominate the PL spectrum. Wells narrower than 3 monolayers exhibit temperature- independent emission and 1 ns radiative lifetimes.

10:12AM H23.00012 Enhancement of Subband Effective Mass in Ag/Ge(111) Thin Film Quantum Wells. SHU-JUNG TANG, WEN-KAI CHANG, Department of Physics and Astronomy, National Tsing Hua University, YU-MEI CHIU, Department of Electrophysics, National Chiao-Tung University, HSIN-YI CHEN, Department of Physics and Astronomy, National Tsing Hua University, CHENG-MAW CHENG, National Synchrotron Radiation Research Center, KU-DING TSUEI1, TOM MILLER, TAI-CHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — Subband dispersions of quantum-well states in Ag films on Ge(111) have been determined by angle-resolved photoemission. The effective masses of the subbands at the zone center increase substantially for decreasing film thicknesses. This peculiar behavior is attributed to a kinetic constraint for standing wave formation governed by a momentum-dependent phase shift function. No evidence is found for in-plane electron localization within the confined geometry.

1National Synchrotron Radiation Research Center
of the nanotubes. We have also observed that the interaction between polyynes and nanotubes is stronger for nanotubes with small diameters.

10:36AM H23.00014 Direct writing of hafnium diboride metallic nanostructures on silicon (100) surfaces using a UHV-STM

WEI YE, University of Illinois at Urbana Champaign, PAMELA MARTIN, NAVNEET KUMAR, JOHN ABELSON, GREG GIROLOMI, ANGUS ROCKETT, JOSEPH LYDING, University of Illinois at Urbana Champaign — The patterning of metallic nanostructures on surfaces is of great interest in fabricating nanoelectronics and quantum devices. In this work, we deposited HfB

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nanostructures on silicon surfaces from Hf(BH

4

)4 by electron beam induced deposition (EBID). At positive sample bias, the electron beam from a STM probe initiates the local CVD by the decomposition of Hf(BH

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)4 under STM tip. By repeatedly scanning STM tip along a specific path, well-defined HfB

2

nanostructures can be directly written onto the surface. Scanning tunneling spectroscopy was used to characterize the electronic properties of the nanostructures. We have achieved 4 nm linewidths and complete selectivity relative to adjacent H-Si(100) regions. The thickness of the nanostructures is controlled by the exposing time to the electron beam from STM tip, while the width is controlled only by the geometry of the tip apex and the sample-tip separation. STS data confirm that the HfB

2

nanostructures deposited are pure metallic, indicating minimum contaminations in the nanostructures, which we attribute to the carbon-free nature of the CVD precursor. To our knowledge this is the first demonstration of sub-5 nm metallic nanostructures in a STM/CVD experiment.

Tuesday, March 17, 2009 8:00AM - 11:00AM – Session H24 DCMP: Focus Session: Chemical Modification of Nanotubes 326

8:00AM H24.00001 Single Molecule Detection in Living Biological Cells using Carbon Nanotube Optical Probes

MICHAEL STRANO, MIT — Nanoscale sensing elements offer promise for single molecule analyte detection in physically or biologically constrained environments. Molecular adsorption can be amplified via modulation of sharp singularities in the electronic density of states that arise from 1D quantum confinement [1]. Single-walled carbon nanotubes (SWNT), as single molecule optical sensors [2-3], offer unique advantages such as photostable near-infrared (n-IR) emission for prolonged detection through biological media, single-molecule sensitivity and, nearly orthogonal optical modes for signal transduction that can be used to identify distinct classes of analytes. Selective binding to the SWNT surface is difficult to engineer [4]. In this lecture, we will briefly review the immersing field of fluorescent diagnostics using band gap emission from SWNT. In recent work, we demonstrate that even a single pair of SWNT provides at least four optical modes that can be modulated to uniquely fingerprint chemical agents by the degree to which they alter either the emission band intensity or wavelength. We validate this identification method in vitro by demonstrating detection and identification of six genotoxic analytes, including chemotherapeutic drugs and reactive oxygen species (ROS), which are spectroscopically differentiated into four distinct classes. We also demonstrate single-molecule sensitivity in detecting hydrogen peroxide, one of the most common genotoxins and an important cellular signal. Finally, we employ our sensing and fingerprinting method of these analytes in real time within live ST3 cells, demonstrating the first multiplexed optical detection from a nanoscale biosensor and the first label-free tool to optically discriminate between genotoxins. We will also discuss our recent efforts to fabricate biomedical sensors for real time detection of glucose and other important physiologically relevant analytes in vivo. The response of embedded SWNT in a swellable hydrogel construct to osmotic pressure gradients will be discussed, as well as its potential as a unique transduction mechanism for a new class of implantable sensors.


ZHENHUI WANG, PETER MORSE, JIANG WEI, OSCAR VILCHES, DAVID COBDEN, University of Washington — We have fabricated mass balances each consisting of an individual single-walled carbon nanotube suspended across a micron-sized trench in an oxidized Si wafer. The vibrational resonance frequency of a nanotube, which is in the range 50-500 MHz, is determined by monitoring the current through it while applying an electrostatic driving signal. The sensitivity of the balances corresponds to just a few atoms. We have compared the monolayer mass shifts due to Ar and Kr, and measured a family of adsorption isotherms on Ar below 77 K. From the latter we calculated the isosteric heat of adsorption on the nanotube surface, which is found to be lower than that of Ar on basal plane graphite and only slightly larger than the latent heat of sublimation of bulk Ar at these temperatures. In one device we observed a phase transition in the adsorbed Ar near monolayer completion. In another device, which probably consists of two nanotubes joined in parallel, we observed enhanced adsorption at lower coverages which may be in the groove between the two nanotubes. This work is supported by the NSF, grant number 0606078.

8:48AM H24.00003 Resonance Raman study of Polynes encapsulated in single-wall Carbon Nanotubes with different diameters

L. G. MOURA, L.M. MALARD, Universidade Federal de Minas Gerais, D. NISHIDE, Nagoya University, Y. ACHIBA, Tokyo Metropolitan University, M. A. PIMENTA, Universidade Federal de Minas Gerais — Polynes are one of the simplest linear carbon chains and they have been recently encapsulated in single-wall carbon nanotubes. The stability of encapsulated polynes opens a way to investigate experimentally these sp-hydrized carbon structures and to study of electronic correlation effects in 1D systems with potential applications in nanoelectronics. In this work we present a resonance Raman study of C10H2 and C12H2 polynes inside single-wall carbon nanotubes with different diameters, using many different laser energies in visible range. We show that the observed optical resonance energies of the polynes depends on the diameter of nanotubes, the maximum of the resonances decreasing with increasing diameter of the nanotubes. Moreover, the resonance energy is generally lower for C12H2 than C10H2. We have also observed a red-shift and strong changes in the shape of Raman G band of the metallic nanotubes when they encapsulate the polynes, and these results were interpreted in terms charge transfer between these two systems and its effect on the electron-phonon coupling of the nanotubes. We have also observed that the interaction between polynes and nanotubes is stronger for nanotubes with small diameters.
The data showed for the doped films the metallic term (linear in $T$) would be as case in a dc conductivity measurement. Also the dc resistance of both B-doped and annealed SWNT films were measured over 10 approach to transparent electrodes. The optical transmission ($T=300K$) of SWNT and B-doped SWNT films measured in the range 50-700 cm$^{-1}$ show that most of these compounds, little charge transfer ($< 0.1$) occurs. Finally, these calculations are compared with results for the adsorption at oxidation defects.

This research was supported by NSF through grant # DMR-0705077.

9:12AM H24.00005 Study of propane films adsorbed on Purified HiPco Carbon Nanotubes1. TOYOHISA FURUSHASHI, DINESH RAWAT, ALDO MIGONE, Department of Physics Southern Illinois University — We investigated the adsorption characteristics of propane on purified HiPco single-walled carbon nanotubes for coverages limited to the first layer. We found two prominent substeps present in the monolayer; this suggests the presence of at least two distinct groups of binding energy sites in the substrate. The results are similar to those that we have found for ethane, but different from those we measured for butane, on the same substrate. We compare and contrast the characteristics of the isotherms for these three alkanes. A high-binding-energy (low-pressure) adsorption isotherm substep is present for all three alkanes. By contrast, the high-pressure substep (corresponding to adsorption on the outer surface area of the nanotubes bundles) shows a gradual smearing with increasing alkane length; this feature is barely resolvable for butane. We also found a gradual increase in the binding energy of alkane molecules with the increasing carbon chain length. This result confirms findings of simulation results for similar systems.

This research was supported by NSF through grant # DMR-0705077.

9:24AM H24.00006 Adsorption of Nitro Aromatics on Single-Walled Carbon Nanotubes, ERIK ALLREDGE, STEFAN BADESCU, THOMAS REINECKE, NAVDEEP BAJWIA, F. KEITH PERKINS, ERIC SNOW, US Naval Research Laboratory — Recent experiments with arrays of carbon nanotubes reveal a strong conductivity response after exposure to aromatic molecules containing nitro functional groups, such as nitrobenzene and trinitrotoluene. The detection of these compounds is of particular interest in the use of nanotube arrays as chemical sensors. To develop an understanding of the microscopic mechanisms involved, we perform detailed ab initio calculations of adsorption geometries, charge configurations, and vibration spectra for these compounds on pristine armchair and zigzag nanotubes. We use density functional theory with localized orbitals in a cluster approach and the M05-2X functional that is appropriate for the weak interactions of physisorption for these systems. We find a strong increase in adsorption energy with the addition of each nitro group to a molecule (around 100 meV) and a gradual increase with nanotube size, in agreement with preliminary experimental results. For most of these compounds, little charge transfer ($< 0.1$ e) occurs. Finally, these calculations are compared with results for the adsorption at oxidation defects.

9:36AM H24.00007 Transparent Boron-Doped Nanotube Films1. XIAOMING LIU, HUGO ROMERO, HUMBERTO GUTIERREZ, PETER EKLUND — We report results of FTIR transmission and temperature-dependent resistance measurements on transparent thin films of bundled single-walled carbon nanotubes exposed to B2O3 at 1000C. This reaction is proposed to B-dope the films. Doping is observed to lower the $T=300 K$ dc sheet resistance by a factor of five without changing the optical transmittance in the visible range and suggests that boron-doped SWNT provide a better approach to transparent electrodes. The optical transmission ($T=300 K$) of SWNT and B-doped SWNT films measured in the range 50-7000 cm$^{-1}$ show that the doped films have a greater optical density in the mid to far IR, consistent with the B-doping creating new free carriers. This optical result shows that the DC conductivity of the doped tubes is indeed higher, with the interpretation not being entangled with changes in the tube-tube contact resistance within the film, as would be the case in a dc conductivity measurement. Also the dc resistance of both B-doped and annealed SWNT films were measured over 10$^2$-300 K. The data showed for the doped films the metallic term (linear in $T$) is $\sim 10$ times greater than for the annealed and undoped films. Work supported by NSF NIRT ECS 06-09243.

1 NSF NIRT ECS 06-09243

9:48AM H24.00008 Kinetic selectivity effects of binary mixtures on nanotube bundles: Internal and external adsorption, SEYOUNG TSIGE, MERCEDES CALBII, JARED BURDE, Southern Illinois University Carbondale — We investigate kinetic selectivity effects that take place during the adsorption of a binary mixture inside a nanotube and on the external surface of a bundle. By using a kinetic Monte Carlo Scheme we allow adsorption on sites with different binding energy (external surface) and we restrict adsorption/desorption only to the end sites in the case of the internal adsorption. In both cases, we analyze the appearance of an overshoot in the fractional coverage of the weaker species (before equilibrium) observed previously for a single, homogeneous, one-dimensional chain.

10:00AM H24.00009 Temperature Programmed Desorption on Carbon Nanotube Bundles: a Computer Simulation study, NAYELI ZUNIGA, MERCEDES CALBI, JARED BURDE, Southern Illinois University Carbondale — We present a study of gas desorption on external surfaces of carbon nanotube bundles by means of a kinetic Monte Carlo scheme. Starting with an initial coverage, we follow the amount of gas desorbed as the temperature increases for different values of initially occupied sites and initial temperature of the sample. We analyze the spectrum obtained in terms of the different binding energies of the adsorption sites. We also compare our results with some available experimental measurements on nanostructure bundles and other nanostructures.

10:12AM H24.00010 Scattering Process of Gas Molecules on Vertically Aligned Single-Walled Carbon Nanotubes, IKUYA KINEFUCHI, YUSHI HARADA, JUNPEI KAWASAKI, KEI ISHIKAWA, SHU TAKAGI, SHIGEO MARUYAMA, YOIYMATOH MATSUMOTO, The University of Tokyo — Scattering process of gas molecules on quartz surfaces covered with vertically aligned single-walled carbon nanotubes (VA-SWNTs) was investigated using the molecular beam technique. We found that the surface modification with VA-SWNT films significantly enhances the energy transfer between gas molecules and surfaces at room temperature and makes the energy accommodation coefficient of helium, which tends to be small even for contaminate surfaces because of the large mass mismatch between helium and surface atom, close to unity. Our results demonstrate a potential application of VA-SWNTs as nanoscale fin structures to enhance heat transfer between gas phase and solid surfaces. As the surface temperature increases, however, the energy accommodation becomes less efficient since the small adsorption energy reduces the trapping probability of helium on carbon nanotube (CNT) bundles. The weak dependence of the accommodation coefficient on the film thickness suggests that gas molecules penetrate into the films because of their high porosity and suffer more than one collision with CNT bundles.
Carbon Nanotube CdSe Nanoparticle Hybrid Materials: Synthesis and Optical Properties. AUSTIN AKEY, CHENGUANG LU. Columbia University, Department of Applied Physics and Applied Math, WEI WANT, Columbia University, Department of Chemistry, IRVING HERMAN, Columbia University, Department of Applied Physics and Applied Math — Carbon nanotubes present remarkable opportunities for the construction of nanomaterials with unique properties, and for use in sensors and optoelectronic device applications. Chemical attachment of nanoparticles to nanotubes has thus far resulted in low loading; direct nucleation of particles on the tube sidewalls leads to a loss of control over particle size and monodispersity. We report the synthesis of novel heterostructures composed of single-walled carbon nanotubes and chemically attached, monodisperse cadmium selenide nanoparticles. Pyridine is used to strip the ligand shell from the nanoparticles, which are then bound to SWNTs in suspension. The resulting hybrid material is stable and resists aggregation; TEM and SEM characterization shows the nanotubes to be densely covered with nanoparticles. The nanoparticles used range in size from 3.5 to 6.0 nm in diameter, and exhibit strong quantum confinement. Also synthesized were hybrids of carbon nanotubes with core-shell CdSe/ZnS nanoparticles and with CdSe nanorods. The absorption and photoluminescence properties of the hybrid materials are also presented.

Electrochemical and Optical Characterization of Metal-Decorated Carbon Nanotubes. TATYANA SHEPS, VAISKUNTH R. KHAPAL, ALEXANDER A. KANE, PHILIP G. COLLINS, Department of Physics and Astronomy, University of California Irvine, Irvine, CA 92697-4576 — HYUNMIN KIM, ERIC O. POTMA, Department of Chemistry, University of California Irvine, Irvine, CA 92697-4576 — Hybrid electrodes combining carbon nanotubes with metal and metal oxide particles are promising for many catalytic applications including energy conversion and energy storage. Understanding the chemical interactions between the nanotube substrate and the catalytic nanoparticle is crucial for optimizing these types of electrodes. Here, we describe techniques for interrogating the metal-nanotube interface on the single-molecule level, using isolated single-walled nanotubes (SWNTs) decorated by single metal particles as the most basic, representative element of a bulk hybrid electrode. The resulting composite and its chemical interface is studied by two complementary techniques, electrochemical voltammetry and Raman spectroscopy. Results comparing the electrochemical behavior with the surface chemistry are presented.


Electrochemical and Optical Characterization of Metal-Decorated Carbon Nanotubes. 

Tuesday, March 17, 2009 8:00AM - 10:48AM
Session H25 DMP: Focus Session: Probing and Modifying Materials with Lasers

Advances in micro/nano scale materials processing by ultrafast lasers. COSTAS FOTAKIS, IESL-FORTH — Materials processing by ultrafast lasers offers several attractive possibilities for micro/nano scale applications based on surface and in bulk laser induced modifications. The origin of these applications lies in the reduction of undesirable thermal effects, the non-equilibrium surface and volume effects coupled with reactive chemical interface, the suppression of photochemical effects in molecular substrates, the possibility of optimizing of energy dissipation by temporal pulse shaping and the exploitation of filamentation effects. Diverse applications will be discussed, including the development and functionalization of laser engineered surfaces, the laser transfer of biomolecules and the functionalization of 3D structures constructed by multiphoton stereolithography. Two examples will be presented in this context: A new approach for the development of superhydrophobic, self-cleaning surfaces [1,2] and the fabrication of functional scaffolds for tissue engineering applications [3-5].

References:

Positional Accuracy in Optical Trap-Assisted Nanolithography. CRAIG B. ARNOLD, EUAN MCLEOD, Princeton University — The ability to directly print patterns on size scales below 100 nm is important for many applications where the production or repair of high resolution and density features are important. Laser-based direct-write methods have the benefit of quickly and easily being able to modify and create structures on existing devices, but feature sizes are conventionally limited by diffraction. In this presentation, we show how to overcome this limit with a new method of probe-based near-field nanopatterning in which we employ a CW laser to optically trap and manipulate dispersed microspheres against a substrate using a 2-d Bessel beam optical trap. A secondary, pulsed nanosecond laser at 355 nm is directed through the bead and used to modify the surface below the microsphere, taking advantage of the near-field enhancement in order to produce materials modification with feature sizes under 100 nm.

3D photofabrication by femtosecond laser pulses and its applications in biomedicine. ALEKSANDR OVSJANIKOV, XIAO SHIZHOU, MANGIRDAS MALINAUSKAS, BORIS CHICHKOV, Laser Zentrum Hannover e.V. — Two-photon polymerization (2PP) is a novel laser-based microstructuring technique. In this approach, the multiphoton absorption of femtosecond laser pulses is used to induce a highly localised chemical reaction leading to a photopolymerization of the material. By moving the laser focus in 3D the trace of modified material is created. In the next step, the unmodified material is removed by an appropriate developer, and the fabricated structure is revealed. Therefore, fabrication of any computer generated 3D structure by “direct laser recording” into the volume of photosensitive material is possible. Nonlinear nature of the interaction allows true 3D microfabrication and realisation of structures with submicrometer resolution. Realistically, we studied possible applications of 2PP in tissue engineering provides possibility to fabricate series of exactly identical scaffolds. Therefore, it is possible to conduct systematic studies of cell interactions in 3D environment. In this contribution, our recent advances in two-photon activated laser processing, properties of applied materials, and applications of this technology are discussed.
9:00AM H25.00004 Single-pulse fabrication of deep vertical nano-holes with a microjoule femtosecond laser.  
LOYD M. DAVIS, YELENA V. WHITE, XIAOXUAN LI, ZBIGNIEW SIKORSKI, WILLIAM H. HOFMEISTER, University of Tennessee Space Institute — When a single energetic 200-femtosecond laser pulse is tightly focused onto the surface of a dielectric material, Zener (tunnelling) ionization and Zener-seeded saturation avalanche ionization cause a plasma to be formed at the surface. The tail of the pulse reflects from the plasma so that the resultant damage is typically shallow. However, we have found that when the laser pulse is focused with negative spherical aberration, holes exceeding 11 microns in depth and with diameters at the surface of only 200—500 nm may be created. A simple acetate sample replication technique is used to estimate the dimensions of the holes. The validity of the replication technique for characterizing such high-aspect-ratio features is confirmed by focused ion-beam sectioning of holes followed by visualization with a scanning electron microscope. We discuss physical processes that may be responsible for the creation of such deep nano-holes, including the role of self-focusing of the laser beam, and the possibility of acceleration of electrons along the direction of the laser beam into the hole. Applications, including direct laser writing of vertical channels for nanofluidic devices, are discussed. Related research on femtosecond laser machining of diamond is also presented.

9:12AM H25.00005 Optical Bulk Metamaterials  
XUANG ZHANG, NSF Nanoscale Science and Engineering Center (NSEC) University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Lab — Metamaterials are artificially designed subwavelength composites that possess extraordinary properties not existing in naturally occurring materials. In particular, they can alter the propagation of electromagnetic waves resulting in negative refraction, sub-wavelength focusing, and transmission of sub-wavelength information over a finite distance. Such unusual properties can be obtained by a careful design of the metal-dielectric composites on a deep sub-wavelength scale. The metamaterials may have profound impact in a wide range of applications such as nano-scale imaging, nanolithography, and integrated nano photonics. I will discuss a few recent experiments demonstrating intriguing phenomena associated with Metamaterials. These include sub-diffraction limit imaging and focusing, low loss negative refraction and imaging in bulk optical metamaterials, and Negative-index Metamaterials (NIM) exhibiting negative phase propagation that can be accessed from free-space. I’ll also discuss nano plasmonics for imaging and bio-sensing.

9:48AM H25.00006 Coloration of single crystal ZnO with ultraviolet laser irradiation1.  
ENAMUL KHAN, S.C. LANGFORD, J.T. DICKINSON, Washington State University — Many dielectric crystals color in the visible region of the spectrum when exposed to intense ultraviolet light such as excimer laser irradiation. In the alkali and alkaline earth halides, the decay of self-trapped excitons produces strongly absorbing defects. We were recently surprised to see single crystal ZnO darken dramatically during exposure to 193-nm ArF excimer laser radiation. ZnO is a wide bandgap (3.44 eV) semiconductor of significant technological interest. The increase in absorption is very broadband, extending from the bandgap into the infrared, and appears nearly black or grey. We present convincing evidence that this color is due to metallic zinc nanoparticles residing on the surface of the irradiated region. As expected, the laser fluence has considerable impact on the size, number, and spatial distribution of these nanoparticles. We propose a model for production of metallic nanoparticles on the surface.

1This work was supported by the US DOE under Grant DE-FG02-04ER-15618.

10:00AM H25.00007 Generation of point defects in femtosecond laser interactions with Cr targets  
EAMAN TAHIR, University of Baghdad, Iraq, ZHIBIN LIN, Texas A&M University, USA, LEONID ZHIGILEI, University of Virginia, USA — The mechanisms and driving forces responsible for the generation of point defects (vacancies and interstitials) in femtosecond laser interactions with Cr target are investigated in atomic-scale simulations. Two series of simulations are performed. In the first set of simulations, the processes induced by 200 fs laser pulse irradiation of a bulk Cr target are studied with a computational model that combines the classical molecular dynamic method with a continuum description of the laser excitation of conduction band electrons, electron-phonon coupling, and electron heat conduction. The distribution of point defects in the surface regions of irradiated targets is analyzed by a broad range of laser fluences, covering the regimes of surface melting, photomechanical spallation, and ablation. To investigate the relative contributions of the thermally-activated generation of vacancy-interstitial pairs and the production of the vacancies during the solidification process, the second series of simulations of solidification at fixed temperatures below the melting point is performed. The densities of vacancies generated under different undercooling conditions are related to the distributions observed in laser-irradiated targets. The implications of the computational predictions for atomic mixing and damage accumulation in multi-pulse irradiation regime are discussed.

10:12AM H25.00008 Nanostructuring of thin gold films by femtosecond laser-induced melt dynamics  
ARSENIY KUZNETSOV, JURGEN KOCH, BORIS CHICHKOV, Laser Zentrum Hannover e.V. — Femtosecond laser irradiation of thin gold films with fluences close to the ablation threshold induces formation of various nanostructures on the film surface [1-3]. These structures are formed due to laser-induced melting of gold and redistribution of the melted material from the edges into the center of the irradiated region. Shape of the created structures can be controlled by varying the laser intensity distribution over the gold film surface. It is shown that the sizes of the produced structures can be below than 100 nm. In this paper, a study of laser-induced molten material dynamics is presented. Analysis of the structural shapes produced with different laser intensity distributions and dynamical reflection measurements allow clarifying mechanisms of the structure formation. Possible applications of this nanostructuring method are discussed.


E. HARO-PONIATOWSKI, Universidad A. Metropolitana Iztapalapa Mexico, J. C. ALONSO-HUITRON, IIM-UNAM-Mexico, C. ACOSTA-ZEPEDA, M. C. ACOSTA-GARCIA, N. BATINA, Universidad A. Metropolitana Iztapalapa — Nanostructured silver thin films in a quasipercolated state are used as the starting morphology for inducing changes in shape and ordering effects by pulsed laser irradiation with a Nd:YAG laser (355 nm) [1,2]. The complex nanostructures are transformed into nanospheres which in turn are ordered in regular patterns when irradiated through a diffractive element such as a slit or a pinhole. The samples are deposited onto TEM grids by the pulsed laser deposition technique. These transformations are subsequently characterized by transmission electron microscopy and by atomic force microscopy. The observed effects are explained using Fresnel diffraction theory. Excellent agreement with the experimental results are obtained. [1] E. Haro-Poniatowski et al. Appl. Phys. Lett. 87, 143103, 2005 [2] E. Haro-Poniatowski et al. Radiation Effects & Defects in Solids 162, 491-499 (2007)
10:36AM H25.00001 Examining Femtosecond Laser Induced Plasma Dynamics via Ultrafast Electron Shadow Imaging1, JUNJIE LI, RICHARD CLINITE, XUAN WANG, JIM CAO, Physics Department/National High Magnetic Field Lab, Florida State University, ZHAOYANG CHEN, SAMUEL MAO, Department of Mechanical Engineering, University of California at Berkeley, JIM CAO TEAM, SAMUEL MAO COLLABORATION — We report a study of the dynamics of plasma creation and evolution in real time using a pulsed electron beam to create two-dimensional shadow images of the plasma plume. Due to the electron beam’s sensitivity to charge, the dynamics of electric fields and charge motion during the earliest stage of laser ablation of Copper plate were directly measured by taking snapshots of the plasma shadow images. Based on a dipole field assumption, a multiplying magnitude of Q(average charge), d(average electrons’ distance from surface), and t(duration of field) is obtained, Q*dt ~ 12*10^-8 *e*m*s, under 6.8*10^14 W/cm^2 laser power on 0.3mm diameter area, moreover, most electrons which are initially emitted retract back in 1 to 2 ps after laser pulse. The results provide new information about multi-photon emission and charge motion during intense laser material interaction.

Tuesday, March 17, 2009 8:00AM - 11:00AM
Session H26 DMP: Focus Session: Graphene IV: Electronic and Structural Properties 328

8:00AM H26.00001 Graphene-based nanomechanical cooling device1, VAN JU LI, DAOXIN YAO, ERICA CARLSON, Purdue University — We propose a novel structure for nanomechanical cooling, based upon graphene. Because thermal transport occurs perpendicular to the surface of the substrate, the proposed structure can be used to facilitate thermal transport between two objects in contact. Furthermore, the strength of the Seebeck coefficient may be tuned by applying pressure. We calculate the Seebeck coefficient in this geometry, as a function of applied voltage and strain.

1The authors acknowledge support from Research Corporation and NSF DMR-0804748

8:12AM H26.00002 Doping Single-Layer Graphene from SiO2 Substrates or Jointed Few-Layer Graphene, LAIN-JONG LI, YUMENG SHI, Nanyang Technological University — Electrostatic force microscopy (EFM) measurements reveal that the surface potential of graphene either increases or decreases, depending on the initial surface potential of substrates, to a “bulk” value with their thickness. Graphene layers tend to screen the substrate potential, which drives the charge exchange between graphene and the substrate. The direct consequence is the effective doping of graphene, where the substrate-dependent p- or n-doping of graphene is corroborated by Raman spectroscopy and electrical measurements for the transistor devices. Our results promise a practical method for tailoring the electronic properties of graphene for nanoelectronics.

8:24AM H26.00003 Graphene-based Materials1, RODNEY RUOFF, The University of Texas at Austin — Our top-down approaches [Lu et al.] inspired physicists to obtain graphene by micromechanical exfoliation. Another approach to individual layers involves converting graphite to graphene oxide (GO) to generate aqueous colloidal suspensions of ‘graphene oxide’(GO) sheets. (i) Reduced GO’ (RGO’) sheets were embedded in polymers such as polystyrene and their dispersion/morphology studied by SEM/TEM, and the conductivity/percolation threshold of such composites was determined; (ii) individual GO’ and RGO’ sheets were studied to elucidate their chemical, optical, and electrical properties, (iii) GO’ and RGO’ sheets were embedded in thin glass films by a sol-gel route yielding conductive/transparent films, (iii) a ‘paper’ material of stacked GO’ sheets was made and characterized, (iv) powders composed of RGO’ showed exceptional promise for use in ultracapacitors, and (v) C13-labeled GO was made and the detailed chemical structure of GO was determined with NMR. –Lu,Yu,Huang,Ruoff, “Tailoring graphite with the goal of achieving single sheets”, Nanotechnology, 10, 269-272 (1999).
See also http://bucky-central.me.utexas.edu/publications.htm 139, 146, 150, 155, 160, 164, 166, 168, 174, 179-182, 184 where collaborators are shown as coauthors.

1Support from NSF, NASA, and DARPA is appreciated.

9:00AM H26.00004 Quantum transport and Klein tunneling in graphene heterojunctions, ANDREA YOUNG, PHILIP KIM, Physics Department, Columbia University — I will discuss the observation of quantum conductance oscillations in extremely narrow graphene heterostructures where a resonant cavity is formed between two electrostatically created bipolar junctions. From analysis of the observed interference pattern, it can be inferred that individual p-n junctions have a collimating effect on transmitted carriers, leading directly to the observation of resonant oscillations despite the largely diffusive carrier dynamics. The oscillatory part of the conductance is insensitive to scattering within individual p-n junctions, electrons which scatter in the junctions, making them a novel probe of the ballistic physics of graphene at the Dirac point and allowing an estimate of the electric field due to nonlinear screening. In a weak applied magnetic field, the oscillations undergo a phase shift characteristic of reflectionless normal transmission, or “Klein Tunneling,” at the individual p-n junctions. Finally, at high magnetic field, graphene heterostructures show modified Shubnikov de Haas oscillations due to the inhomogenous external potential.

9:12AM H26.00005 Electronic transport properties of graphene irradiated by charged particles1, JIAN-HAO CHEN, WILLIAM CULLEN, CHAUN JANG, MICHAEL FUHRER, ELLEN WILLIAMS, Materials Research Science and Engineering Center, Center for Nanophysics and Advanced Materials, Dept of Physics, Univ. of Maryland, College Park, MD — We have measured the effect of low energy charged particle irradiation (electrons, He ions, Ne ions or Ar ions) on the electronic transport properties of clean graphene devices on SiO2. Charged particle irradiation induces additional scattering which is consistent with adding both short-ranged (i.e. point defect) and long-ranged (i.e. charged) impurities to the device. We also performed temperature-dependent conductivity of the irradiated devices from 9K to 400K in ultra high vacuum. In sharp contrast to graphene with charged impurity disorder, which remains metallic at low temperature, even a small amount of irradiation-induced disorder (one order of magnitude increase in room-temperature resistivity compared to pristine devices) produces a divergence of the resistivity and insulating behavior at low temperature for carrier densities below 4*10^{12} cm^{-2}.

1This work was supported by the University of Maryland MRSEC and the Nanoelectronics Research Initiative of the Semiconductor Research Corporation.

9:24AM H26.00006 Fractionalization in graphene-like systems, CONAN WEEKS, UBC, MARCEL FRANZ, University of British Columbia — I will discuss the possible interaction-driven instabilities that can arise in a system of masles Dirac fermions modeled by the extended Hubbard model on the π flux square lattice and the honeycomb lattice, and their relevance to fractionalization in 2D graphene-like systems. Through numerical studies we have shown that these instabilities can result in a number of interesting phases. In addition to the charge density wave and various stripe phases these include the exotic “quantum anomalous Hall” (Haldane) phase and the dimerized “Kekulé” phase. A self consistent calculation inside the Kekulé phase on the π flux lattice indicates that a discretized U(1) vortex can be stabilized in this region leading to a zero-energy bound state with fractional charge e/2.
The conductance of the GNR at the charge neutrality point was suppressed at low temperature, which suggests the opening of an energy gap due to the lateral modulation on the number of graphene layers. An 800-nm-wide bar-shaped device fabricated in single-layer graphene exhibits the half-integer quantum Hall bilayer, and multilayer graphene using tapping-mode atomic force microscope (AFM). We found that the width of the insulating oxidized area depends systematically on the position of the sample for different crystal periodicities. Such observations provide information about the stacking and domain boundaries in epitaxially-grown graphene.

In particular, we studied the evolution of the electronic structure of graphene nanoflakes with very high aspect ratios. Possible mechanisms of graphite exfoliation and graphene nanoribbon formation will be discussed.

\[ \Delta \varphi = \Delta \varphi_0 + \Delta \varphi_1, \]
8:00AM H27.00001 Temperature Dependence of Single-Asperity Friction for Diamond on Diamond and DLC Interfaces1 , C. DUNCKLE, University of California, Irvine, I.B. ALTFEDER, Air Force Research Laboratory, P. TABOREK, University of California, Irvine — A variable temperature, ultrahigh vacuum atomic force microscope with a diamond-coated probe was used to characterize interfacial friction over a temperature range of 30 to 300 Kelvin. A vertical scan was used to measure tip to surface adhesion and contact normal forces. Friction (lateral) force measurements were taken by dragging the tip along the surface. Calibration was done in situ using substrates with known dimensions and angles. Measurements were made on diamond-like carbon surface and a single crystallite in a micro crystalline diamond film. Results were analyzed by fitting into the DMT continuum model. Comparison of friction versus load showed approximately a factor of two increase in the friction at cryogenic temperatures compared to room temperature. Results are qualitatively consistent with MD simulations but are not well described by models of thermally activated friction. Problems associated with temperature gradients at the tip- surface interface will be discussed.

1This work is supported by Extreme Friction: MURI AFOSR # FA9550-04-1-0381.

8:12AM H27.00002 Small amplitude vibrations of curved atomic force microscope cantilevers: Theory , ARVIND NARAYANASWAMY, CARLO CANETTA, NING GU, Columbia University — The shifts in resonance frequencies of cantilevers are used to infer tip–sample interactions in tapping–mode atomic force microscopy as well as in a wide variety of cantilever based sensors. In this work, we investigate theoretically as well as experimentally the effect of curvature on the vibration dynamics of micro–cantilevers to which a micro–sphere is attached at the free end. We show that resonance frequency shifts of cantilevers to which a tip mass is attached can be altered by controlling the curvature of the cantilever. This control over the resonance frequency spectrum is independent of other causes of resonance frequency variation, such as adsorbed mass on cantilever or variation of material properties due to change in temperature. In the case when the cantilever is a bi–material cantilever, this shift in resonance frequency can be used as to detect changes in the thermal environment of the cantilever.

8:24AM H27.00003 Intermodulation Atomic Force Microscopy and Spectroscopy , CARSTEN HUTTER, Stockholm University, DANIEL PLATZ, ERIK THOLEN, DAVID HAVILAND, Royal Institute of Technology, HANS HANSSON, Stockholm University — We present a powerful new method of dynamic AFM, which allows to gain far more information about the tip-surface interaction than standard amplitude or phase imaging, while scanning at comparable speed. Our method, called intermodulation atomic force microscopy (ImAFM), employs the manifestly nonlinear phenomenon of intermodulation to extract information about tip-surface forces. ImAFM uses one eigenmode of a mechanical resonator, the latter driven at two frequencies to produce many spectral peaks near its resonace, where sensitivity is highest [1]. We furthermore present a protocol for decoding the combined information encoded in the spectrum of intermodulation peaks. Our theoretical framework suggests methods to enhance the gained information by using a different parameter regime as compared to Ref. [1]. We also discuss strategies for solving the inverse problem, i.e., for extracting the nonlinear tip-surface interaction from the response, also naming limitations of our theoretical analysis. We will further report on latest progress to experimentally employ our new protocol.


8:36AM H27.00004 Independent determination of depth and energy of electronic trap states in dielectric films by Dynamic Tunneling Force Microscopy , JON PAUL JOHNSON, CLAYTON C. WILLIAMS, University of Utah, Physics Department — Dynamic Tunneling Force Microscopy (DTFM) is a new scanning probe technique that images electronic states in completely non-conducting films with sub-nanometer spatial resolution1. In DTFM, electrons are shuttled via quantum tunneling between a metallic tip and localized electronic states in an insulating dielectric film, while a lock-in amplifier detects an electrostatic force signal that is proportional to the shuttled charge. The DTFM signal provides a map of the available electronic states within tunneling range of the surface. These states are not observable by STM. The depth of the states can be estimated from the dependence of tunneling rate on the tip/sample gap2 and also inferred from their apparent lateral size. Image shows states below the surface that drop out of the image when the tip/sample gap is increased. A methodology is introduced to independently determine state energy and depth, potentially on a sub-nanometer scale. This work was supported by AFOSR and SRC. [1] J P Johnson and C C Williams, Nanotechnology (accepted) [2] N Zheng, et al., Journ. App. Phys. 101, 093702

8:48AM H27.00005 Applications of AFM for atomic manipulation and spectroscopy , OSCAR CUSTANCE, National Institute for Materials Science — Since the first demonstration of atom-by-atom assembly [1], atomic manipulation with scanning tunneling microscopy has yielded stunning realizations in nanoscience. A new exciting panorama has been recently opened with the possibility of manipulating atoms at surfaces using atomic force microscopy (AFM) [2-5]. In this talk, we will present two different approaches that enable patterning structures at semiconductor surfaces by manipulating individual atoms with AFM and at room temperature [2, 3]. We will discuss the physics behind each protocol through the analysis of the measured forces associated with these manipulations [3-5]. Another challenging issue in scanning probe microscopy is the ability to disclose the local chemical composition of a multi-element system at atomic level. Here, we will introduce a single-atom chemical identification method, which is based on detecting the forces between the outermost atom of the AFM tip and the atoms at a surface [6]. We demonstrate this identification procedure on a particularly challenging system, where any discrimination attempt based solely on topographic measurements would be impossible to achieve.

References:

9:24AM H27.00006 Design of a variable temperatures scanning force microscope , E. NAZARETSKI, K. S. GRAHAM, J. D. THOMPSON, J. K. BALDWIN, Los Alamos National Laboratory, J. A. WRIGHT, University of California Los Angeles, D. V. PELEKHOV, P. C. HAMMEL, Ohio State University, R. MOVSITCHOVICH, Los Alamos National Laboratory — We have developed the variable temperature scanning force microscope capable of performing both magnetic resonance force microscopy (MRFM) and magnetic force microscopy (MFM) measurements in the temperature range between 5 and 300 K. Modular design, large scanning area, and interferometric detection of the cantilever deflection make it a sensitive, easy to operate and reliable instrument suitable for studies of the dynamic and static magnetization in various systems. We have verified the performance of the microscope by imaging microfabricated permalloy dots and vortices in Nb thin film in the MFM mode of operation. MRFM spectra in a diphenyl-picryl-hydrazyl film were recorded to evaluate the MRFM mode of operation.
9:36AM H27.00007 Bimodal atomic force microscopy imaging of isolated antibodies in air and liquids. JOSE R. LOZANO, ELENA T. HERRUZO, NICOLAS F. MARTINEZ, RICARDO GARCIA, Inst. Microelectronics Madrid -CSIC, FORCETOOL TEAM — We develop a dynamic atomic force microscopy (AFM) method based on the simultaneous excitation of the first two flexural modes of the cantilever. The instrument, called bimodal AFM, opens up additional channels (amplitude and phase of the 2

9:48AM H27.00008 High-Resolution Magnetic Resonance Force Microscopy using Iron Filled Carbon Nanotubes. MICHAEL HERMAN, PALASH BANERJEE, KIN CHUNG FONG, DENIS PELEKHOV, The Ohio State University, FRANZISKA WOLNY, THOMAS MUHL, BERND BUCHNER, Leibniz Institute for Solid State and Materials Research, CHRIS HAMMEL, The Ohio State University — Magnetic Resonance Force Microscopy is able to probe below surfaces to map out spins in a non-destructive manner by measuring the force from the dipolar coupling of a magnetic probe to spins in the sample. We have used low force constant cantilevers with low intrinsic dissipation to obtain 2 spin sensitivity. To obtain better sensitivity one avenue of improvement is to increase the magnetic field gradient from the magnetic probe. Iron-filled carbon nanotubes provide a promising route for very high magnetic field gradient micromagnetic probes; we have successfully attached these iron nanowires to IBM style ultrasoft silicon cantilevers. The smaller size of the tip (15 to 25 nm) allows gradients an order of magnitude greater than micron-sized rare-earth magnets. In addition, iron filled carbon nanotubes also exhibit high anisotropy fields, a result of the shape anisotropy. This work was supported by the Army Research Office under W911NF-07-1-0305 and the National Science Foundation under DMR-0807093.

10:00AM H27.00009 Electron Spin Magnetic Resonance Force Microscopy of Nitroxide Spin Labels. ERIC W. MOORE, SANGGAP LEE, STEVEN A. HICKMAN, SARAH J. WRIGHT, JOHN A. MAROHN, Department of Chemistry and Chemical Biology, Cornell University — Nitroxide spin labels are widely used in electron spin resonance studies of biological and polymeric systems. Magnetic resonance force microscopy (MRFM) is a magnetic resonance technique that couples the high spatial resolution of a scanning probe microscope with the species specificity of magnetic resonance. We report on our investigations of 4-amino TEMPO, a nitroxide spin label, by force-gradient MRFM. Our microscope operates at high vacuum in liquid helium, using a custom fabricated ultra-soft silicon cantilever in the magnet-on-cantilever geometry. An 18 T gap coupled microstrip line resonator supplies the transverse field.

10:12AM H27.00010 A Compact, Wide Temperature Range (300mK-300K) Magnetic Force Microscope using High Resolution Fibre Interferometer and Alignment-Free Cantilevers. OZGUR KARCII, NanoMagnetic Instruments Ltd., MUNIR DEDE, Bilkent University, AHMET ORAL, Sabanci University, NANOMAGNETICS INSTRUMENTS TEAM, BILKENT UNIVERSITY COLLABORATION, SABANCI UNIVERSITY COLLABORATION — We describe a design of a Low Temperature Magnetic Force Microscope (LT-MFM) for variable temperatures between milli-Kelvin temperatures to 300 K. The design of LT-MFM is very compact, 23.6mm ODx200mm, flexible and is compatible with almost any cryostat (included PPMS of Quantum Design Inc), even He3 systems or DR, provided that there is enough space. The sensor is mounted on a scan piezo tube which has five quadrants: four quadrants are used for scanning, the fifth electrode is used for dithering the cantilever by means of a digital Phase Lock Loop (PLL) with 5mHz frequency resolution. We employed a fibre interferometer deflection measurement for our LT-MFM. A special alignment holder is designed for this purpose. A 225µm length MFM cantilever is placed on an Alignment-Free AFM Cantilever holder chip from NanoSensors. Our design can sustain cantilever-fiber alignment down to 300mK without any signal loss. An improved fiber interferometer with ~1x10^{-3} A/Hz noise level is designed and used to detect cantilever deflection. LT-MFM also enables us to work under high external magnetic fields.


10:36AM H27.00012 Development of Superconducting Quantum Interference Device DC Magnetometer for High Magnetic Field and Dilution Refrigerator Applications. J.-H. PARK, T.P. MURPHY, S.W. TOZER, E.C. PALM, National High Magnetic Field Laboratory, FSU, Tallahassee, FL — A commercially available SQUID (Superconducting Quantum Interference Device) DC magnetometer is often limited by its relatively high temperature (≥ 1.9 K) and low magnetic field (≤ 7 T) operating environment. The need for the lower temperature and higher field DC magnetization measurements keeps growing as more materials show interesting physical phenomena whose energy scales are relevant to low temperatures (~ mk). To meet these needs we have developed a probe for a top loading dilution refrigerator in which all the DC magnetometer components including SQUID electronics, detection coil, and sample motion shaft are placed together. The probe was tested in a top loading dilution refrigerator and the results show that the base temperature at 25 mK increased ~ 1.6 % when the sample displacement was 3.2 cm with a speed of 3 cm/min. The moment of the test sample was successfully detected down to 50 mK. Improvement in coil balancing and shielding of the detection coil are planned.

1 This work was supported by NSF-DMR-0084173, DOE-DE-FG52-06NA26193, and an IHRP at the NHMFL.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H28 DMP FIAP: Focus Session: Thermolectric Materials: Transport Physics
shells leads to the low thermal conductivities experimentally measured \[1\]. We consequently successfully compare the results of our calculations \[3\] with the magnitude of the isotope effect on the thermal conductivities of carbon and boron nitride single-walled nanotubes \[2\]. We furthermore show that intershell carbon nanotubes \[1\]. Using an ab initio atomistic Green's function approach, we demonstrate that localization cannot be observed in the thermal conductivity of isotope-disordered boron nitride and carbon nanotubes \[1\].

The difficulty associated with thermoelectric materials is the need to couple and optimize a variety of physical properties which determine the thermoelectric efficiency. The parameters of a thermionic device featuring a doped diamond material as the emitter electrode to maximize the output power produced. For example, a TEC operating between $900 \, ^\circ\text{C}$ and $300 \, ^\circ\text{K}$ with an emitter negative electron affinity of $0.5 \, \text{eV}$, a collector barrier height of $0.6 \, \text{eV}$, Richardson's constant of both electrodes equal to $10 \, \text{Acm}^{-2} \text{K}^{-2}$, emissivity of both electrode of $0.5$, and interelectrode spacing of $10 \, \mu\text{m}$ will have a maximum output power of $1.5 \, \text{Wcm}^{-2}$ and efficiency of $20\%$ occurring at an emitter barrier height of $1.2 \, \text{eV}$. The efficiency calculation includes electronic and blackbody heat transport across the device. The analysis establishes approaches to increase the efficiency to values greater than $20\%$. This work was funded by the Office of Naval Research through the TEC MURI Program.

**8:36AM H28.00002 Nanostructured materials design for thermoelectric applications**, KEIVAN ESFARJANI, MONA ZEBARJADI, ALI SHAKOURI, University of California at Berkeley — Nanostructured materials have shown great promise for superior thermoelectric properties. Recently, our collaborators and us have been able to enhance thermoelectric properties of InGaAs by doping it with ErAs nanoparticles. Transport properties are dominated by scattering of electrons with nanoparticles, phonons and impurities. We can design the scattering potential of the former to maximize the power factor, P is in fact an inverse problem, attempting to solve for the best nanoparticle scattering potential which maximizes P. Using a least square method, we find the potential which minimizes the difference between the actual scattering cross section and its target value. The target value is chosen so as to display energy filtering property. More generally, we also simply maximize the power factor with respect to the nanoparticle potential profile. A simple and fixed model is chosen for other scattering rates, as well as the dispersion relation for the bulk electrons results between the two approaches will be compared in order to see the effect of electron filtering property on the power factor enhancement.

**8:48AM H28.00003 Influence of Dimensionality on Thermoelectric Device Performance**\[1\] . RASEONG KIM, Purdue University, SUPRIYO DATTA, MARK S. LUNDSTROM — Significant improvements in the thermoelectric figure of merit have recently been demonstrated in low dimensional structures. These improvements have been largely due to the reduced lattice thermal conductivity, so the question of how much additional improvement is possible by engineering the electronic structure has become important. Our goal is to present a clear answer to this question using the Landauer formalism, which applies from the ballistic to diffusive limits. We first relate thermoelectric coefficients to the transmission and the number of conducting channels, M(E). The optimum M(E) is known to be a delta-function. We then compare thermoelectric coefficients in one, two, and three dimensions and show that the channels are utilized more effectively in lower dimensions. The shape of M(E) improves as dimensionality decreases, but lower dimensionality itself does not guarantee better performance because it is controlled by both the shape and the magnitude of M(E). To realize the advantage of lower dimensionality, the packing density must be more effectively in lower dimensions. The shape of M(E) improves as dimensionality decreases, but lower dimensionality itself does not guarantee better performance because it is controlled by both the shape and the magnitude of M(E). To realize the advantage of lower dimensionality, the packing density must be more effectively in lower dimensions.

**9:00AM H28.00004 Optimized vacuum thermionic energy conversion using diamond materials**, JOSHUA SMITH, Carnegie Mellon University, GRIFF BILBRO, North Carolina State University, ROBERT NEMANICH, Arizona State University — The vacuum thermionic energy conversion device (TEC) has been an attractive alternative to other means of energy production for some time due to its potentially high efficiency operation, but practical devices have been difficult to develop as a result of the low net space charge effect. It is well known that a hydrogen termination layer on a diamond material induces a negative electron affinity (NEA). In this study we present a theoretical analysis showing it is possible to tune the parameters of a thermionic device featuring a doped diamond material as the emitter electrode to maximize the output power produced. For example, a TEC operating between $900 \, ^\circ\text{K}$ and $300 \, ^\circ\text{K}$ with an emitter negative electron affinity of $0.5 \, \text{eV}$, a collector barrier height of $0.6 \, \text{eV}$, Richardson's constant of both electrodes equal to $10 \, \text{Acm}^{-2} \text{K}^{-2}$, emissivity of both electrode of $0.5$, and interelectrode spacing of $10 \, \mu\text{m}$ will have a maximum output power of $1.5 \, \text{Wcm}^{-2}$ and efficiency of $20\%$ occurring at an emitter barrier height of $1.2 \, \text{eV}$. The efficiency calculation includes electronic and blackbody heat transport across the device. The analysis establishes approaches to increase the efficiency to values greater than $20\%$. This work was funded by the Office of Naval Research through the TEC MURI Program.

**9:12AM H28.00005 Nanostructured Silicon as a Thermoelectric Material**, ARUNAVA MAJUMDAR, University of California at Berkeley — No abstract available.

**9:48AM H28.00006 Design of thermoelectric composite materials for energy applications**, MARTIN MALDOVAN, EDWIN THOMAS, Massachusetts Institute of Technology — Energy supply is becoming a major world-wide problem as fossil energy supplies decrease while energy demands increase. Thermoelectric materials, which reversibly convert thermal and electrical energy, offer the prospect of power generation and cooling by means of the rational transport of electrons and phonons. In nanocomposite materials, both quantum and classical effects provide opportunities to control the transfer of electrons and phonons. The difficulty associated with thermoelectric materials is the need to couple and optimize a variety of physical properties in order to exhibit necessary efficiencies, which are determined by the figure of merit ZT. To exhibit large efficiencies, the best thermoelectric material should possess low thermal conductivity (similar to that of a glass) and high electrical conductivity (similar to that of a perfect crystal material). In this paper we study thermoelectric materials by preparing composite materials that can provide the desired coupled physical properties. Our research concentrates on predicting and designing thermoelectric material properties using theoretical and computational methodologies. We use currently available algorithms with numerical techniques to design thermoelectric materials with increased efficiencies. The ultimate goal of our research is to develop a basic understanding of the coupled physical properties in these materials and to create a framework that allows for the systematic design, optimization, and characterization of their thermal and electric properties.

**10:00AM H28.00007 Thermal conduction mechanisms in isotope-disordered boron nitride and carbon nanotubes**, IVANA SAVIC, NATALIO MINGO, LITEN, CEA-Grenoble, France, DEREK STEWART, Cornell Nanoscale Facility, Cornell University, USA — We present first principles studies which determine dominant effects limiting the heat conduction in isotope-disordered boron nitride and carbon nanotubes \[1\]. Using an ab initio atomistic Green's function approach, we demonstrate that localization cannot be observed in the thermal conductivity of isotope-disordered boron nitride and carbon nanotubes \[1\]. 


1This work was supported by the National Science Foundation under grant number ECS- 0609282.

**8:00AM H28.00001 Thermoelectricity: A Bottom-up View**, SUPRIYO DATTA, Purdue University — It is well-known that the nature of electronic transport changes significantly as the length L of the active region of a device is reduced from millimeter down to nanometer dimensions. Historically our understanding of electrical resistance and conduction has progressed top-down: from large macroscopic conductors to small atomistic conductors. Indeed thirty years ago it was common to argue about what, if anything, the concept of resistance meant on an atomic scale. Since then there has been significant progress in our understanding, spurred by actual experimental measurements made possible by the technology of miniaturization. However, despite this progress in understanding the flow of current on an atomic scale, the standard approach to the problem of electronic transport continues to be top-down and we have argued elsewhere that an alternative bottom-up viewpoint can be extremely illuminating \[1\]. In this talk we will briefly summarize this viewpoint and discuss the unique insights it provides into the subject of thermoelectricity and thermoelectric device design in general and into the possibilities of molecular thermoelectrics in particular.

Title: Phonon relaxation times extracted from first principles thermal conductivity calculations

Authors: D. A. BROIDO, A. WARD, Department of Physics, Boston College, Chestnut Hill, MA 02467

Abstract: The lattice thermal conductivity of semiconductors, κ_L, is a key component in assessing a material's utility for thermoelectric applications. Calculations of κ_L commonly employ phonon relaxation times, τ_pkh. Over the past few decades, a variety of mathematical forms have been used for these τ_pkh to represent the phonon-phonon scattering [1], which dominates the behavior of κ_L around and above room temperature. However, these forms have typically been obtained in a low frequency/low temperature approximation where umklapp scattering is weak and outside the thermal regime of interest for thermoelectrics. Recently we have developed a first principles approach that accurately calculates κ_L using no adjustable parameters [2]. In this presentation, we use our ab initio results for Si, Ge and diamond to examine the accuracy of the different models for τ_pkh, and we identify alternative models. [1] See for example, M. Asen-Falmer et al., Phys. Rev. B 56, 9431 (1997), and references therein. [2] D. A. Broido, M. Malorny, G. Birner, N. Mingo and D. A. Stewart, Appl. Phys. Lett. 91, 231922 (2007).

1 (Supported by NSF)

Title: Intrinsic lattice thermal conductivity of diamond from first principles

Authors: A. WARD, D. A., BROIDO, Department of Physics, Boston College, Chestnut Hill, MA, 02467, D. A. STEWART, Cornell Nanoscale Facility, Cornell University, Ithaca, NY, 14853


2 (Supported by NSF)

Title: Thermal boundary resistance of closely-spaced Si/Ge interfaces from lattice dynamics calculations

Authors: ERIC LANDRY, ALAN MCGAUGHEY, Carnegie Mellon University

Abstract: An ability to accurately predict the thermal boundary resistance (TBR) of closely-spaced semiconductor interfaces will allow the design of superlattices with high values of the thermoelectric figure-of-merit. Here, the TBR and phonon transmission coefficients of closely-spaced Si/Ge interfaces are predicted using harmonic lattice dynamics calculations and the scattering boundary method. The atomic interactions are modeled using the Stillinger-Weber potential. The computational domain contains a thin germanium layer sandwiched between two semi-infinite extents of silicon, forming two closely-spaced interfaces. We also consider the opposite situation, where a silicon layer is placed between two large extents of germanium. Due to the harmonic approximation, the calculations are only valid when the phonon scattering is elastic. To examine the assumption of elastic scattering, we compare the lattice dynamics predictions to those obtained using molecular dynamics simulations and the direct method, which require no assumptions about the nature of the phonon transport. We conclude by discussing how the atomic force constants needed in the lattice dynamics calculations can be calculated from density functional theory. This novel approach will allow for the prediction of TBR for interfaces between semiconductors for which a suitable interatomic potential does not exist.

Title: Prediction of phonon transport properties and thermal conductivities in superlattices by anharmonic lattice dynamics calculations

Authors: JOSEPH TURNEY, ALAN MCGAUGHEY, Carnegie Mellon University, CRISTINA AMON, University of Toronto

Abstract: Phonon transport in superlattices is investigated using anharmonic and quasi-harmonic lattice dynamics calculations. Within the lattice dynamics framework, we develop a method for predicting the properties of both coherent and incoherent phonons. The method is implemented for test systems consisting of Stillinger-Weber silicon-germanium superlattices. In these systems the mode dependent frequencies, heat capacities, group velocities, transmission coefficients, and relaxation times of the phonons are computed and used to predict the thermal conductivity. We relate changes in the superlattice structure (e.g., period length and interface roughness) to the predicted phonon properties and, for each structure, identify the phonon modes that dominate thermal transport.

Tuesday, March 17, 2009 8:00AM - 9:48AM – Session H29 FEd: The Physics and Astronomy New Faculty Workshops II

Title: How the New Faculty Workshop in 2004 affected my teaching-learning strategies

Authors: NATALIA DUSHKINA, Department of Physics, Millersville University

Abstract: In this presentation, I will discuss how my experience with the New Faculty Workshop in fall 2004 affected my course offering and teaching-learning strategies in PHYS 103, PHYS 132 and PHYS 331: Fundamentals of Optics courses. PHYS 103, Elements of Physics, is a general education conceptual physics lab course with no prerequisites for non-science majors. PHYS 331, Fundamentals of Optics, is a lab-based course required for physics majors, which was offered for the first time at the MU Department of Physics in fall 2007. I will discuss curricular changes, as well as new teaching-learning and assessment methods implemented in these courses for the first time at our department. I will offer examples of peer group discussions, just in time teaching and the effect of chapter summaries on motivating the students and their participation in problem solving.

3 APS

Title: Taking inquiry to the next level: Tablet PC’s to stimulate active learning and unify introductory physics curriculum

Authors: TIKHON BYKOV, Physics Department, McMurry University, Abilene, TX 79697, YELENA KOSHElevA, Psychology Department, McMurry University, Abilene, TX 79697

Abstract: Tablet PC’s have been adapted to student peer group discussions. Student feedback showed that modifications were beneficial. Student knowledge assessment, performed with the FCI test, indicated improvement in student learning.
success at UCF during the initial phase of the project. R. Thornton, and P. Laws which has met with success at other universities and colleges. It was recently been adopted at the University of Central Florida (UCF), a large metropolitan university that is rapidly becoming a major research university. A key question is then if successful physics education practices

8:36AM H29.00004 How Physics Test Scores Reflect the Students’ Time Spent, MARIA BABUC-HAMILTON, Marshall University, Huntington, WV, TIM HAMILTON, Shawnee State University, Portsmouth, OH — We found that exam scores in introductory physics courses show a wedge-shaped pattern when plotted against the order they are turned in. The article will explore some of the factors contributing to this pattern and will propose guidelines to help determine an ideal test time limit, aimed at students with good perseverance and average skill. The reason for this pattern appears to stem from a combination of students’ skills and perseverance. The first students to finish tend to have either the best or worst grades in the class, with few in between. Students with the highest skills (knowledge, memory, problem-solving skills) need little time to finish, and they have the confidence to turn in the test quickly, before other students. Good students with moderately high skills tend to take longer. The later submissions gradually converge to a grade close the class average. Results of over 200 grades from students in different introductory physics classes, from two universities, taught using a variety of methods, when collected and analyzed, show the same wedge-shaped pattern. This seems to indicate a universal component of the pattern, which does not depend on the teaching methods or the test structure. From our analysis, we aim at deriving what an ideal test time limit would be, at which students hit a point of diminishing returns.

8:48AM H29.00005 “Physical Concepts in Cell Biology,” an upper level interdisciplinary course in cell biophysics/mathematical biology, DIMITRIOS VAVYLONIS, Department of Physics. Lehigh University — I will describe my experience in developing an interdisciplinary biophysics course addressed to students at the upper undergraduate and graduate level, in collaboration with colleagues in physics and biology. The students had a background in physics, biology and engineering, and for many the course was their first exposure to interdisciplinary topics. The course did not depend on a formal knowledge of equilibrium statistical mechanics. Instead, the approach was based on dynamics. I used diffusion as a universal “long time” law to illustrate scaling concepts. The importance of statistics and proper counting of states/paths was introduced by calculating the maximum accuracy with which bacteria can measure the concentration of diffuse chemicals. The use of quantitative concepts and methods was introduced through specific biological examples, focusing on model organisms and extremes at the cell level. Examples included microtubule dynamic instability, the search and capture model, molecular motor cooperativity in muscle cells, mitotic spindle oscillations in C. elegans, polymerization forces and propulsion of pathogenic bacteria, Brownian ratchets, bacterial cell division and MinD oscillations.

9:00AM H29.00006 The Quality Enhancement Plan Matrix (12 years and still tweaking the process!), GARY MANKEY, University of Alabama — As an alumni of the 1997 New Faculty Workshop, I’ve had plenty of opportunities to experiment with the teaching methods introduced there. Most recently, faculty at UA have been asked to develop a Learner-Centered approach to teaching, where regular, timely and thorough assessment of student learning becomes a key component of the curriculum. This involves four phases: 1) Identifying and defining learning outcomes, 2) Matching assessments to outcomes, 3) Identifying baselines and progression toward benchmarks and 4) Documenting the process using a quality enhancement plan matrix. This has led to the development of learning tools designed to enhance critical thinking and problem solving skills. This will be discussed in the context of setting teaching goals for new faculty, including how to document the process for teaching portfolios.

9:12AM H29.00007 Pedagogical Reforms from Private Engineering to Public University, LOK LEW YAN VOON, WSU — This talk will document my and associated colleagues’ impact on physics pedagogy at the two universities I have been employed at from my initiation at the New Faculty Workshop as an assistant professor in 1998 to being currently a full professor and chair. The present reforms involving our introductory physics courses are connected to our science education program.

9:24AM H29.00008 Applying Hands-On Activity Concepts to Advanced Mathematical Instruction for Physics, WILLIAM DIETERLE, California University of Pennsylvania — While the use of hands-on instruction by constructivist principles has been extensively documented and is covered in great detail in the New Faculty Workshops run by APS, most examples discussed in this series apply to the introductory course level. Many of the same principles can be applied at the upper division level, but topics that are normally considered purely mathematical do not readily lend themselves to such an approach. A common complaint of students first studying vector analysis in an upper division course is the fact that they can’t relate the divergence, curl, and gradient to real life. This talk discusses a method of presentation emphasizing the physical significance of these mathematical entities, with laboratory exercises for a two-dimensional gradient and for the divergence theorem in three dimensions. The approach has been successfully utilized in the first weeks of an upper division electricity and magnetism class.

9:36AM H29.00009 Meeting the Challenges of New Faculty – My Own Lesson, MIRELA FETEA, University of Richmond — A few years ago, I thought that students with different scientific backgrounds posed the biggest challenge for me – a new assistant professor teaching physics courses at a small liberal-arts private college. I thought that my knowledge of physics, enthusiasm, and willingness to succeed are most of the ingredients needed to become a very good teacher – how little I knew... Now, after being awarded tenure, having received a Distinguished Educator Award, an Outstanding Mentor award, and serving as acting-chair in my department, I am grateful for having had the opportunity to attend The Physics and Astronomy New Faculty Workshop which is responsible for who I am today. This presentation will offer a reflection on how the teaching techniques presented by specialists in pedagogy or educational methodology at The Physics and Astronomy New Faculty Workshop shaped my own performance as a teacher.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H30 DMP GMAG: Focus Session: Superconducting and Magnetic Oxide Superlattices and Films 334
8:00AM H30.00001 Magnetism in Complex Oxide Heterostructures Determined with Neutron Scattering 1, SUZANNE G.E. TE VELTHUIS, Argonne National Laboratory — With the creation of high quality superlattices consisting of complex oxide materials novel materials exhibiting a wide range of interesting phenomena are emerging. Due to the diverse physical properties of complex oxides, (e.g., ferromagnetism, antiferromagnetism, superconductivity), some of which can be varied by doping, the versatility in their applications is large. The physical properties in these new materials, often is tied to the behavior at the interfaces between the different components of the superlattice, and therefore requires detailed knowledge of the relationship between the chemical and electronic composition. Polarized neutron reflectometry (PNR) provides access to the depth-dependent magnitude and orientation of the magnetization and can therefore link the magnetic to the electronic and chemical properties, especially close to these transitions. Antiferromagnetism, ferromagnetism, and superconductivity, some of which can be varied by doping, the versatility in their applications is large. The physical properties in these new materials, often is tied to the behavior at the interfaces between the different components of the superlattice, and therefore requires detailed knowledge of the relationship between the chemical and electronic composition. Polarized neutron reflectometry (PNR) provides access to the depth-dependent magnitude and orientation of the magnetization and can therefore link the magnetic to the electronic and chemical properties, especially close to these transitions.

8:36AM H30.00002 Spatial Mapping of the Interface Orbital Reconstruction in LaCaMnO$_3$/YBa$_2$Cu$_3$O$_7$ Heterostructures, J.W. FREELAND, E. KRATSOV, Advanced Photon Source, Argonne National Laboratory, S. GRENIER, J.-M. TONNERRE, Institute Neel, C.N.R.S., Grenoble, France, M. KAREEV, J. LIU, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville — Interfaces between strongly correlated electron materials is an exciting area for exploring new phenomena as these states are altered in the proximity of the interface. In recent work, we have shown that at the interface between the ferromagnetic metal LaCaMnO$_3$ and the superconductor YBa$_2$Cu$_3$O$_7$ the electronic state of Cu undergoes an orbital reconstruction[1,2]. Here we present results using polarization-dependent resonant scattering at the Cu L edge to probe depth dependence of the orbital occupancies in the YBCO layer. By modeling the scattering in the region of the YBCO (001) Bragg peak in LCMO/YBCO heterostructures, we can work to extract a picture of the orbital occupancies in the interface region. Work at Argonne is supported by the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357. JC is funded by U.S. DOD-ARO under Contract No. 0402-17291.

8:48AM H30.00003 Electronic and Magnetic Properties of the Interface Between a High-Tc Cuprate and CMR Manganese, JIAN LIU, University of Arkansas, J. FREELAND, B. KIRBY, M. KAREEV, H.U. HABERMEIER, G. CRISTIANI, J. CHAKHALIAN — Atomically controlled interfaces between two materials can give rise to novel physical phenomena and functionalities. Modern synthesis methods have yielded high-quality hetero-junctions of oxide materials with competing order parameters. Orbital reconstructions and covariant bonding has been shown to be important factors in the rational design of oxide heterostructures[1]. To clarify the role of superconductivity we study the interface between a high-temperature superconductor (Pr$_2$B$_2$Cu$_3$O$_7$ and CMR manganite La$_2$/3Cu$_1$/3Mn$_3$O$_7$ by resonant x-ray spectroscopy, magneto-optics and neutron reflectivity. The resulting data provide a hint of orbital changes and strong modification of magnetic structure in the heterojunction. 1. J. Chakhalian et al, Science, v. 318, 1155 (2007).

9:00AM H30.00004 Dynamics of Proximate Order Parameters Measured by the Time-Resolved Magneto-Optical Kerr Effect in SrRuO$_3$/YBa$_2$Cu$_3$O$_7$ Heterostructures, C.L.S. KANTNER, M.C. LANGNER, Dept. of Physics, UC Berkeley and Lawrence Berkeley National Lab, S.P. CRANE, L.W. MARTIN, Y.-H. CHU, P. YU, Dept. of Materials Science, UC Berkeley, R. RAMESH, Dept. of Physics and Dept. of Materials Science, UC Berkeley, J.W. ORENSTEIN, Dept. of Physics, UC Berkeley and Lawrence Berkeley National Lab — The interaction between ferromagnetic and superconducting complex oxides in a heterostructure is a subject of great interest. This recent observation of ferromagnetic resonance in SrRuO$_3$ by the time-resolved magneto-optical Kerr effect (TRMOKE) presents a new method for insight into such a system. TRMOKE has been used to compare the temperature dependence of magnetization dynamics in SrRuO$_3$ grown on insulating substrates and ferromagnetic SrRuO$_3$/superconducting YBa$_2$Cu$_3$O$_7$ heterostructures. The substantial differences between SRO grown on an insulating substrate compared to YBCO as well as the effects seen upon passing through the YBCO transition temperature are reported.

9:12AM H30.00005 Competition between high Tc superconductivity and ferromagnetism in oxide multilayers, CHRISTIAN BERNHARD, University of Fribourg and Fribourg Center for Nanomaterials — Artificial multilayers offer unique opportunities for combining materials with antagonistic orders such as superconductivity and ferromagnetism. It was previously shown for multilayers of classical superconductors and ferromagnets that fascinating new quantum states can be realized by tuning the layer thicknesses or the interface properties. In my talk, I will show that multilayers of cuprate high Tc superconductors (HTSC) in oxide-based ferromagnets provide an equally fascinating playground for studying the competition between the superconducting and ferromagnetic orders under the condition that both opponents are of comparable strength. I will present experimental results from neutron reflectometry and low energy muon spin rotation (LR) measurements on thin film superlattices that were grown by pulsed laser deposition (PLD). These measurements establish that the interaction between superconductivity and ferromagnetism is surprisingly strong and gives rise to a number of unexpected and very unusual phenomena. In particular, our data provide evidence that a giant superconductivity-induced modulation of the vertical profile of the ferromagnetic magnetization takes place in some of these superlattices.

9:48AM H30.00006 Enhanced Superconductivity in Superlattices of High-Tc Cuprates, SATOSHI OKAMOTO, THOMAS MAIER, Oak Ridge National Laboratory — We investigate the electronic properties of multilayers of strongly correlated models for cuprate superconductors using cluster dynamical mean-field techniques. We focus on combinations of underdoped and overdoped layers and find that the superconducting order parameter in the overdoped layers is enhanced by the proximity effect of the strong pairing scale originating from the underdoped layers. The enhanced order parameter can even exceed the maximum value in uniform systems. This behavior is well reproduced in slave-boson mean-field calculations which also find higher transition temperatures than in the uniform system. This work was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy. A portion of this research at Oak Ridge National Laboratory’s Center for Nanophase Materials Sciences was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.
10:00AM H30.00007 Anomalous Expansion of the Cu-Apical O Distance in Superconducting Cuprate Oxide Bilayers , HUA ZHOU, National Synchrotron Light Source, Brookhaven National Lab, YIZHAK YACOB, Racah Institute of Physics, Hebrew University, RONALD PINDAK, National Synchrotron Light Source, Brookhaven National Lab, VLADIMIR BUTLER, DAVID G. HUDDLESTON, IVAN BOZOVIC, CMPMS Department, Brookhaven National Lab — Interfaces between complex oxides have received considerable attention due to the observation of fascinating quasi two- dimensional phenomena such as a high-mobility electron gas, interfacial ferromagnetism, and, recently, the observation of interfacial high-temperature superconductivity in epitaxially grown bilayers of metallic La0.55Sr0.45CuO4 and insulating La2CuO4 on LaSrAlO4 substrates.

To help understand the mechanism underlying the observed interfacial superconductivity, we directly measured the 3D electron density of this epitaxial bilayer, C.S. TUREL, T.L. WU, J.Y.T. WEI, University of Toronto, I.J. GUILARAN, P. XIONG, Florida State University — Andreev reflection has been extensively used to determine the spin polarization of various ferromagnetic materials, with conventional two-terminal measurements in magnetic fields of up to 12 Tesla were performed on thin film vanadium dioxide (VO2), ALEXANDRA A. FURSINA, Department of Chemistry, Rice University, 6100 Main st. Houston, TX, 77005, R.G. SUMESH SOFIN, IGOR V. SHVETS, CRANN, School of Physics, Trinity College, Dublin 2, Ireland, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University, 6100 Main st. Houston, TX, 77005 — Magnetite, Fe3O4, is an example of strongly electronically correlated system. It undergoes so called Verwey transition at TV ≈ 122 K accompanied both by structural distortion and drastic decrease in electrical conductivity, i.e. metal-insulator transition. Recently, we discovered a new electrically driven phase transition in magnetite nanoparticles and thin films. We observed that a low-temperature (T < TV) insulating state is broken upon applying an electric field, resulting in a sharp transition to the state with much higher conductivity. We report on further electrical characterization of this newly discovered state. There is a question whether this state is the same as high-temperature phase above Tc, or this is a new state of magnetite. In standard two-terminal measurement dominant contribution of contact resistance impedes intrinsic electrical properties. Thus, four-terminal configuration is necessary. Electrical and magnetoresistance properties are measured in challenging four-terminal geometry at nanoscale.

1 Funding for this research was provided by the Center for Emergent Materials at the Ohio State University, a NSF MRSEC (Award Number DMR-0820414).

10:24AM H30.00009 Magnetic and structural properties of half-metallic Sr2FeMoO6 epitaxial films fabricated by ultra-high vacuum sputtering1, ADAM HAUSER, R.A. RICCIARDO, A. GENC, R.E. WILLIAMS, P.M. WOODWARD, H.L. FRASER, F.Y. YANG, The Ohio State University — Sr2FeMoO6, a double-perovskite half-metallic ferromagnet, has attracted much attention because of its high Tc of 420 K. However, the fabrication of Sr2FeMoO6 epitaxial films has been challenging due to impurity phases and disorder. Using ultrahigh vacuum off-axis RF sputtering with precisely controlled low-concentration H2 in Ar, we have fabricated phase-pure Sr2FeMoO6 epitaxial films on SrTiO3 (001) and (111) substrates. X-ray diffraction confirms pure phase with double perovskite ordering. The phase purity and magnetic moments are highly sensitive to the H2 partial pressure. The optimal range for the H2 concentration is 0.4% to 0.6% in Ar with 70 mTorr total pressure. The saturation magnetization of the Sr2FeMoO6 films grown in this range is 1.5 μB/Fe per formula unit at 5 K, which is a strong magnetization considering the epitaxial strain. Aberration-corrected HAADF TEM images reveal atomically sharp interface between Sr2FeMoO6 and SrTiO3.

1 Supported by DOE DE-FG02-06ER46328

10:36AM H30.00010 Atomic structure of the polar Fe2O3(0001)/MgO(111) interface1, K. PANDE, M. GAJARDZISKA-JOSIFOVSKA, M. WEINERT, U. Wisconsin—Milwaukee — We present a first-principles investigation of the stability and structural properties of layer-by-layer growth of thin films of Fe2O3(0001) (hematite) on polar MgO(111). The interface is "oxide-like," atomically abrupt, and stabilized by significant structural relaxations. The electronic and magnetic properties are found to vary as a function of hematite film thickness. In contrast to the insulating and antiferromagnetic nature of bulk hematite, the heterointerface is half-metallic and ferromagnetic. Drastic structural rearrangements of the Fe2O3 overlay are observed at a critical thickness of three Fe bilayers, resulting in an effective expulsion of oxygen from the hematite film. To clarify the effect of the MgO(111) substrate polarity on the nature and growth of the Fe2O3 films, comparisons will be made to unsupported hematite slabs and to Fe2O3/Ti(0001) interfaces.

1 Supported by DOE DE-FG02-06ER46337.
8:12AM H31.00002 Mott metal-insulator transition-induced electrical oscillation in VO₂, HYUN-TAK KIM, ETRI, YONG WOOK LEE, Pukyong University; ETRI, BONG-JUN KIM, SUN JIN YUN, ETRI, SONGYOUL CHOI, BYUNG-GYU CHAE, ETRI — Since Mott predicted the abrupt first-order metal-insulator transition (MIT) in 1949, one of the most important issues in contemporary solid-state physics has been to experimentally prove Mott’s MIT in a strongly correlated system with electron-electron interaction. The MIT has many practical applications and is believed to facilitate the understanding of physical phenomena, such as high-Tc superconductivity, colossal magnetoresistance, etc. In particular, in order to reveal the mechanism of the Mott MIT, many physicists have paid attention to a representative paramagnetic insulator, VO₂(4d³), with an abrupt resistance change near 68°C. The key issue is whether VO₂ is a Mott insulator, in which the abrupt MIT is not caused by a structural phase transition (SPT), or a Peierls insulator undergoing the SPT near Tₜₚₓ ≈ 68°C; this question can be answered when a monoclinic and correlated metal (MCM) phase different from a normal metal is observed. Here we show an MCM phase, high frequency electrical oscillations in the MCM phase of VO₂. The oscillation possibly is generated from a temporal capacitor, which is comprised of both temporary dielectric components, arising from inhomogeneity in a VO₂ film, and MCM phases acting like electrodes. This work concluded that the electrical oscillation is a characteristic of the Mott MIT. (Ref: Applied Physics Letters 92 (2008) 162903).

8:24AM H31.00003 De-coupling Electrical and Thermal Effects in Triggering Metal-Insulator Transition in VO₂ Thin Film Devices, GOKUL GOPALAKRISHNAN, SHRIRAM RAMANATHAN, School of Engineering and Applied Science, Harvard University — Vanadium dioxide (VO₂) has been shown to undergo an abrupt electronic phase transition near 70°C from a semiconductor to a metal, with an increase in dc conductivity of over three orders of magnitude, making it an interesting candidate for advanced electronics as well as for fundamental research into understanding the Mott transition. Recent experiments strongly suggest that this transition can be manifested independent of a structural phase transition in the system at a similar temperature, and that it can be triggered by the application of a critical field across the VO₂ thin film. To address the important question of thermal effects due to the applied field, we report the results of electro-thermal simulations on a number of common and promising device geometries showing the extent of heating caused by the leakage current in the “off” state of the VO₂ device. The simulation results are compared with experimentally observed device characteristics. Valuable insights into the nature of the metal-insulator transition can be obtained from such simulations and will be discussed in the presentation.

8:36AM H31.00004 Properties of Complex Oxides at the Nanoscale: First Order Phase Transitions through Avalanches, 1, AMOS SHARONI, Department of Physics, UC San Diego — Properties of complex oxides have been studied for decades, including many systems which exhibit a phase transition, among which are high temperature superconductors, multiferroics, and metal insulator (M-I) transition materials. We have studied a member of the later group, vanadium oxide (VO₂), which in spite of its long history, keeps surprising researchers today. We find that the M-I transition of nano-scaled VO₂ devices is drastically different from the smooth transition curves generally reported. The temperature driven M-I transition occurs through a series of resistance jumps ranging over two decades in magnitude, indicating that the transition between the two phases of the system happens by resistive avalanches. The avalanche magnitude follows statistically a power law similar to that observed in many other physical systems, such as Barkhausen noise in ferromagnets or sand avalanches in sand piles, and nonphysical systems such as connectivity of the internet. We discuss the effects on the distribution of avalanches due to the: device dimensions, percolative nature of the measurement and interactions between the different phases within the phase transition. We present additional evidence for the importance of interactions in macroscopic FORC measurements, and their role in the opening of the hysteresis in VO₂ M-I transitions.

1Work done in collaboration with J. G. Ramirez, Y. Dubi, M. E. Gomez and I. K. Schuller and funded by the U.S. Department of Energy and the AFOSR.

9:12AM H31.00005 FORC Analysis of the thermal hysteresis at the Metal Insulator Transition in VO₂, JUAN RAMIREZ, Universidad del Valle, Cali-Colombia, AMOS SHARONI, JONATHAN DUBI, University of California, San Diego, MARIA E. GOMEZ, Universidad del Valle, Cali-Colombia, IVAN K. SCHULLER, University of California, San Diego — We use the first order reversal curve method (FORC) to characterize the metal-insulator phase transition in VO₂ thin films. By studying the hysteresis properties of resistance vs. temperature we were able to obtain information regarding inter-domain interactions. An unexpected tail like feature in the contour plot of the FORC distribution indicates the existence of irreversible regions outside of the hysteresis loop. This irreversibility may arise from metallic domains present at various temperatures below the closing of the hysteresis, which interact with the surrounding medium and change the reversal path relative to one coming from a fully insulating state. We develop a model where the driving force which opens hysteresis in VO₂ is inter-domain interactions. This model is intrinsically different from the Preisach model that is usually used to describe hysteresis, since it identifies a microscopic origin of the hysteresis, and provides physical parameters to characterize it. Work Supported by the US Department of Energy, AFOSR and the Colombian agencies COLCIENCIAS and the Excellence Center for Novel Materials, CENM.

9:24AM H31.00006 Electric field effects on phase transition and electronic transport mechanisms in vanadium oxide thin films, CHANGHYUN KO, SHRIRAM RAMANATHAN, Harvard University — Metal-insulator transitions (MIT) in complex oxide thin films are of great interest from both scientific and application perspectives. Vanadium oxide is a model system to exploit strongly correlated electronic phenomena such as Mott transition. Furthermore, wide attention for application has been attracted by its transition functionality that can be tuned in terms of various external parameters: temperature, electric field, photocexcitation, and stress. The tunable conduction states allow creating novel devices whose functions are controlled by multiple parameters. We report on recent observations of electric-field assisted phase transition in vanadium oxide thin films. The conduction mechanisms were analyzed using both in-plane and out-of-plane modes and matched well. In the insulator phase, Poole-Frenkel emission was suggested to govern non-ohmic behavior at high field regime, while under low field application, ohmic conduction with activation energy of ~0.24 eV was observed. Activation energy of ohmic conduction in the metallic phase was ~0.08 eV. These preliminary results are encouraging towards exploring correlated oxides for computing device technologies.

1The authors acknowledge AFOSR and IQSE, Harvard for financial support.

9:36AM H31.00007 Conductivity Dynamics in the Correlated Metallic State of V₂O₃, M. LIU, B. PARDO, Boston University, Dept. of Physics, M.M. QAZILBASH, UCSD, Dept. of Physics, S.J. YUN, B.G. CHAE, B.J. KIM, H.T. KIM, Electronics and Telecommunications Research Institute, Korea, D.N. BASOV, UCSD, Dept. of Physics, R.D. AVERITT, Boston University, Dept. of Physics — V₂O₃ is a strongly correlated electron material that undergoes a transition from antiferromagnetic insulator at low temperatures to a strongly correlated metal above ~140K. We report on time resolved spectroscopic studies of V₂O₃ thin films where we have observed coherent oscillations in the far-infrared conductivity following excitation with a 35-fs optical pulse. The resultant ~100 ps conductivity oscillations result from the optically induced generation of strain which modulates the orbital overlap and hence the conductivity thus revealing a strong coupling of carriers to the lattice in the metallic state. This contrasts with other vanadates such as VO₂ where this effect is not observed. We will discuss the potential of V₂O₃ as a candidate material for investigating photoinduced phase transitions.
Subdomain studies of the metal-insulator transition in VO$_2$ nanobeams
JIAW WEI, JAE HYUNG PARK, JACOB BEEdle, ZENGHUI WANG, WEI CHEN, GEETA YADAV, DAVID COBDEN, Department of Physics, University of Washington — In many correlated materials, domain structure causes the bulk properties to differ from those on the sub-domain level. In addition, near first-order phase transitions it leads to transition broadening, hysteresis, and sample degradation. Studies of nanoscale crystals enable investigations of the domain-free homogeneous material. We demonstrate this by working with nanobeams of vanadium dioxide, thereby discovering or clarifying multiple aspects of its famous metal-insulator transition at 67°C. Amongst them are that the transition to the metal occurs at a constant value of the resistivity of the insulating phase; large supercooling of the homogeneous metallic phase is possible; and the activation energy in the insulating phase is consistent with the optical gap, in contrast with earlier reports on bulk samples. The nanobeams also enable new classes of experiments, including investigating a single metal-insulator interface wall, employing nanomechanical effects to determine the equilibrium transition temperature, and investigating the dynamics of a phase transition in quasi-one-dimensional geometry.

This work was supported by the Army Research Office.

Infrared nano-imaging of metallic and insulating domains in single crystalline vanadium dioxide nanowires
ANDREW JONES, JIAW WEI, DAVID COBDEN, MARKUS RASCHKE, University of Washington — Correlated electron systems are often associated with heterogeneous electronic and structural phase transitions with ordering and domain formation on nanometer length scales. Vanadium Dioxide (VO$_2$) has long been a material of research focus due to behavior associated with its temperature induced metal-insulator transition (MIT) occurring around 340K. The underlying mechanism of this transition is thought to be the result of a complex interplay between the lattice and electronic degrees of freedom as the material passes through the MIT, whose origin is as of yet poorly understood. We study the nanometer scale formation of insulating and metallic domains of single crystal VO$_2$ nanowires bonded to silica substrate using infrared scattering-scanning near field optical microscopy (s-SNOM). Imaging contrast is obtained due to the distinct optical dielectric properties of the respective metallic and insulating phases. A hierarchy of domain sizes is observed, suggesting two distinct insulating phases in addition to the metallic phase as the material moves through the MIT.

Mapping the spatial scale of domain switching in heteroepitaxial vanadium dioxide thin films and nanoparticles
JOYEE NAG, RICHARD HAGLUND, Vanderbilt University — Vanadium dioxide is a strongly correlated electron system exhibiting a hysteresis semiconductor-to-metal transition around 67°C, accompanied by a structural change from monoclinic to tetragonal and huge changes in its electrical conductivity and near-infrared transmission. As interest grows in very thin films and nanoparticles of vanadium dioxide, the spatial scale and domain structure of the metal-insulator transition are critical issues. To elucidate these questions, thin films and nanoparticles of vanadium dioxide were grown on R-, C- and A-cut sapphire substrates, and the substrate-dependent epitaxial growth habits and in-and-out-of-plane orientations were characterized by near-infrared transmission, X-ray diffraction, scanning and transmission electron microscopy. Temperature variable XRD scans at intervals of one degree were performed from the onset to the completion of the transition hysteresis to map out the percentage of coexisting domains of monoclinic and tetragonal phases in one such 100nm thick epitaxial film.

Self-Limiting Growth of Magnetic Nanoparticles in a Glassy Matrix
SERGIO PICOZZI, MARK LAURENZI III, IAN PEGG, Department of Physics and Vitreous State Laboratory, The Catholic University of America, Washington, DC — Nanoparticles of magnetite can be grown by heat treatment of suitable glass compositions slightly above the glass transition temperature. We have investigated the transformation kinetics and magnetic properties, including the size dependence of the Verwey transition, in such systems. The initially rapid growth is quickly arrested leading to tight size distributions that become essentially independent of time. The mean size (a few nm) is dependent on the glass composition and temperature. In this paper, we investigate a simple model in which the self-limiting nature of this process is ascribed to the experimentally observed strong dependence of the glass transition temperature of the matrix on the concentration of one of the diffusing species, which in turn gives rise to a concentration-dependent diffusivity. In addition, the relationship between the equilibrium concentration of the diffusing species and the curvature of the particle-matrix interface (the Gibbs-Thomson effect) is shown to play a prominent role. The model reproduces the essential features of the transformation kinetics, predicting an initial power law growth that becomes nearly logarithmic at long times, and identifies the key physical parameters that determine the self-limited particle size.

Unusual electronic states in TiO$_2$/VO$_2$ (001) multilayers
VICTOR PARDO, WARREN PICKETT, University of California Davis, PARD0-PICKETT COLLABORATION — Abrupt interfaces between oxides display a wealth of unexpected behavior, and the interface between a band insulator and a Mott insulator is expected to display extra richness. Several multilayered TiO$_2$/VO$_2$ structures have been studied by ab initio density functional theory techniques, including the thin VO$_2$ regime corresponding to the quantum confined Mott insulator. VO$_2$ undergoes a metal-insulator transition near room temperature, but when deposited in thin films of thickness smaller than 5 nm, the metal-insulator transition disappears. Our calculations (using the correlated LDA+U method with modest values of U and J) show that the electronic character (metallic versus insulating) changes with the number of VO$_2$ layers embedded within insulating TiO$_2$ layers: metallic for five VO$_2$ layers, semimetallic and half-metallic for three layers, and insulating for a single VO$_2$ layer. These trends, and the peculiar nature of the three VO$_2$ layer case, will be discussed in some detail.
8:00AM H32.00001 Longitudinal spin fluctuations in itinerant ferromagnets, ANDREI RUBAN, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm — Finite-temperature properties of magnetic materials strongly depend on their magnetic configuration given by relative orientation of local magnetic moments. In itinerant ferromagnets, an additional degree of freedom becomes important: the value of local magnetic moment, which is sensitive to the magnetic state and the local chemical environment of atoms as well as the thermal electronic excitations of different type, leading to the so-called longitudinal spin fluctuations (LSF). LSF play an important role in itinerant magnetic systems at high temperatures. In particular, they are responsible for the existence of finite local magnetic moments on atoms in the paramagnetic state, which affect different physical properties. At the same time, an ab initio based description of the LSF is problematic. The LSF are ignored in the local density and related approximations of density functional theory, which for instance leads to a substantial underestimation or complete disappearance of the local magnetic moments on atoms in the itinerant ferromagnets in the corresponding calculations at high temperature in the paramagnetic state. Although the LSF can be included in more elaborate schemes, such as the dynamical mean-field theory, the application of such techniques to real systems is too cumbersome in most cases. In this work a generalized form of classical magnetic Hamiltonian is suggested, which includes both transverse and longitudinal spin fluctuations on equal footing. Parameters of the Hamiltonian can be determined in the first-principles calculations, within the local spin density approximation. The method is applied to the calculations of high-temperature magnetic properties of Co, Fe and Ni, including the Curie temperature. The effect of the LSF in the high-temperature paramagnetic state on chemical interactions and other physical properties is demonstrated for several alloys, including fcc Fe-Cr-Ni alloys, which is the basis of austenitic stainless steels.

8:36AM H32.00002 Spin excitations in solids from first principles, ARNO SCHINDLMAYR, Department Physik, Universitaet Paderborn, Germany, ERSOY SASIOGLU, MANFRED NIESERT, CHRISTOPF FRIEDRICH, STEFAN BLÜGEL, Forschungszentrum Juelich, Germany — The long-range order of the electron spins in magnetic solids gives rise to additional excitation modes that preserve the charge density but change the total spin of the electron system. While Stoner excitations, which correspond to spin-flip transitions between the majority and minority channels, can be described within a single-particle picture, spin waves are collective modes that result from the spin-dependent exchange interaction between the electrons. Here we discuss different approaches that we have explored for material-specific spin-wave calculations from first principles. All of these methods focus on the non-local and dynamic transverse spin susceptibility, whose spectral function can be directly related to experimental spectroscopies, but employ either time-dependent density-functional theory or many-body perturbation theory to treat exchange and correlation. In the latter case, maximally localized Wannier orbitals are used to efficiently obtain the electron-hole vertex of the multiple-scattering $T$ matrix, which is constructed with full frequency and wave-vector dependence. The implementation uses the full-polarized linearized augmented-plane-wave (FLAPW) method. For ferromagnetic transition metals like Fe, Co or Ni our results are in good agreement with experimental data and reproduce all important spectral features.

8:48AM H32.00003 Transverse spin susceptibility in Ni, Fe and Co, LIQIN KE, TAKAO KOTANI, MARK VAN SCHILFGAARDE, School of Materials, Arizona State University, Tempe, AZ, 85287-8706, VLADIMIR ANTROPOV, Ames Laboratory, Ames, IA, 50011, USA — We calculate the full transverse spin susceptibility $\chi^{\pm}(q,\omega)$ in the time-dependent local density approximation (TDLDA) for elemental Ni, Fe and Co. We extract the Heisenberg exchange constant from both the energy-dependent $\chi^\pm$ and the static one. The results are compared with those given by a method assuming the rigid rotation of the magnetic moments at each site (ref.kotani2008). We observe some differences between these two methods, especially around the Brillouin zone boundaries. We also calculate $\chi^{\pm}$ starting from the non-interacting Hamiltonian generated from the quasiparticle self-consistent GW (QSGW) approximation (ref.kotani2007). We analyze how the QSGW potential alter the LDA results.

9:00AM H32.00004 Ab-initio electronic structure calculations of periodic systems in the presence of arbitrary magnetic fields1, ALFREDO A. CORREA, EUNSEOK LEE, WEI CAI, Department of Mechanical Engineering, Stanford University, GIULIA GALLI, UC Davis — Ab-initio electronic structure calculations in the presence of magnetic fields have been mainly performed for isolated systems, or, in the case of periodic systems, by adopting perturbative approaches. Building on a recent formulation of electronic structure calculations in the presence of magnetic fields [1,2], we will discuss calculations for periodic systems under arbitrary conditions, which include arbitrary (finite) magnetic field, arbitrary periodic cell shapes, and arbitrary magnetic field spatial variations. Preliminary results based on a plane-wave numerical approach and local approximations to Density Functional Theory will be presented.[1] W.Cai, G.Galli, Phys. Rev. Lett. 92, 186402 (2004).[2] E. Lee, W. Cai, G. Galli, J. Comput. Phys. 226, 1310 (2007).

1The work is supported by the DOE/SciDAC project on Quantum Simulations of Materials and Nanostructures.

9:12AM H32.00005 Real space first-principles derived semiempirical pseudopotentials applied to tunneling magnetoresistance1, KIRK BEVAN, Oak Ridge National Laboratory, Materials Science and Technology Division, TONY LOW, Purdue University, Department of Electrical and Computer Engineering, HONG GUO, McGill University, Centre for the Physics of Materials and Department of Physics — We present a real space density functional theory (DFT) localized basis set semi-empirical pseudopotential (SEP) approach. The method is applied to iron and magnesium oxide, where bulk SEP and local spin density approximation (LSDA) band structure calculations are shown to agree within approximately 0.1 eV. Subsequently we investigate the qualitative transferability of bulk derived SEPs to Fe/MgO/Fe tunnel junctions. We find that the SEP method is particularly well suited to address the tight binding transferability problem because the transferability error at the interface can be characterized not only in orbital space (via the interface local density of states) but also in real space (via the system potential). To achieve a quantitative parameterization, we introduce the notion of ghost semi-empirical pseudopotentials extracted from the first-principles calculated Fe/MgO bonding interface. In general the results underscore the need for separate tight binding interface and bulk parameter sets when modeling conduction through thin heterojunctions on the nanoscale.

1Supported by DMSE/BES of DOE and NSF

9:24AM H32.00006 Rational Design of Half-Metallic Alloys1, WILLIAM BUTLER, CLAUDIA MEWES, CHUN-SHENG LIU, MINT Center, University of Alabama, MAIRBEK CHSHIEV, Spintec — A half-metal is a material that is a metal for one spin-channel and an insulator or semiconductor in the other. Half-metals are potentially important for spintronic applications such as magnetic sensors for hard drives and magnetic random access memory. We show using very simple ideas that it is possible to rationally design a class of magnetic alloys by placing a gap at the center of one of the d-bands and placing the Fermi energy in this gap. We will present design rules that can be used to make an infinite number of half-metallic heterostructures. We will also show how the half-metallic feature may be maintained at surfaces and interfaces.

1Work Supported by NSF-DMR-0213985 and by the Information Storage Industry Consortium
9:36AM H32.00007 Density-functional theory study of the Co$_2$MnSi/MgO interface. BJÖRN HÜLSEN, Fritz-Haber-Institut der MPG, PETER KRATZER, University Duisburg-Essen, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Magnetic memory devices that exploit the tunneling magnetoresistance (TMR) effect depend crucially on the spin polarization of the electrode materials. Using ferromagnetic half-metals, such as the full Heusler alloy Co$_2$MnSi, perfect electrodes with 100% spin polarization could possibly be realized, at least at zero temperature. Here, we use density functional theory (DFT) calculations to model an epitaxially grown Co$_2$MnSi/MgO(001) interface in a prospective TMR device. The stability, the electronic and magnetic properties of different terminations of Co$_2$MnSi (stoichiometric Co- and MnSi- and non-stoichiometric Mn- and Si-planes) and different registry with respect to the insulating barrier (Mg-top, O-top, bridge and hollow site) are investigated. We find that the electronic and magnetic properties (including the existence of the spin gap) depend strongly on the termination. The formation energy of the various interfaces is presented in form of a phase diagram. Both the interface Co/O (Co at O top site) with a high spin polarization of $P = 70\%$, and the interface MnSi/O with only small $P$ form part of the thermodynamically accessible region. The MnMn/O interface preserves the half-metallicity of the bulk, but is found to be only metastable. Interface band structures are presented, and magnetic moments are compared to experimental data.

9:48AM H32.00008 Magneto-electric polarizability and axion electrodynamics in crystalline insulators. ANDREW ESSIN, JOEL MOORE, University of California, Berkeley, DAVID VANDERBILT, Rutgers University — Spin-orbit coupling can lead in two- and three-dimensional solids to time-reversal-invariant insulating phases that are “topological” in the same sense as the integer quantum Hall effect and similarly have protected edge or surface states. The three-dimensional topological insulator is known to have unusual magnetoelectric properties referred to as “axion electrodynamics”: it supports an electromagnetic coupling $\Delta E_{el} = (\theta e^2/2\hbar)c - B \cdot \nu$ with $\theta$ as the integer quantum of axial charge. An approach to $\theta$ in any three-dimensional crystal is developed based on the Berry-phase theory of polarization: $\theta e^2/2\hbar c$ is the bulk orbital magnetic polarizability (the polarization induced by an applied magnetic field). We compute the orbital magnetoelectric polarizability for a simple model and show that it predicts the fractional part of surface $\tau_{xy}$, computed using a slab geometry. Although $\theta$ is not quantized once time-reversal and inversion symmetries are broken, it remains a bulk quantity for the same reasons as ordinary polarization.

10:00AM H32.00009 ABSTRACT WITHDRAWN

10:12AM H32.00010 Flexomagnetic effect in Mn-based antiperovskites. RENAT SABIRIANOV, PAVEL LUKASHEV, University of Nebraska at Omaha — We report our theoretical results on the induced magnetization appearance in antiferromagnetic antiperovskites, such as Mn$_3$GaN, due to the gradient of applied external strain (flexomagnetic effect). We model the external flexure by forming a 40-atom Mn$_2$GaN$_2$ supercell with 4 domains under external strain gradient. This structure shows a net magnetization which increases parabolically up to 0.03$\mu_B$ (per Mn atom) in the (0,1,1) direction reflecting non-linear contribution to local piezomagnetic effect in the considered range of up to 0.005% external strain gradient. The calculated flexomagnetic effect is found to be relatively small with induced magnetic moment order of magnitude smaller than that of piezomagnetic contribution. The flexomagnetic effect can be especially important in the nanostructures, where the stress gradients are usually large due to the surface tension. All calculations were performed using the projector augmented wave method.

10:24AM H32.00011 Layered antiferromagnetism with high Neel temperature in the intermetallic compound Mn$_2$Au. SERGIY KHMELEVSKYI, PETER MOHN, Center for Computational Materials Science, Vienna University of Technology, CEMS TEAM — On the basis of earlier experimental studies the intermetallic compound Mn$_2$Au has been characterized as a non-magnetically ordered material. Here we report the results of first-principles calculations based on Local Spin-Density Approximation which describe Mn$_2$Au to have a narrow band antiferromagnetic ground state with rigid local moments on the Mn sites. Calculations of the inter-atomic exchange constants based on the magnetic force theorem and a Monte-Carlo modeling of the resulting Heisenberg-like Hamiltonian predict a very high Neel-temperature of $\sim$1580K. This temperature is considerably higher than for the other known high temperature antiferromagnetic Li$_2$-type Mn based binary alloys, which are widely used in magnetic storage applications. In particular, the source of the difficulties in determining magnetic order from the earlier experiments is discussed. The observed meta-magnetic like behavior and a susceptibility anomaly at low temperatures are linked to the frustrated magnetism on Mn anti-site impurities. We believe that the high temperature antiferromagnetism of Mn$_2$Au may have quite an impact in technology. In particular, it can be considered as a candidate for the application as a “pinning” layer in GMR devices.

10:36AM H32.00012 3d impurities in wide gap oxides—magnetism and carrier doping. HANNAE RAEBIGER, NREL, Golden, CO and Yokohama National University, Yokohama, JAPAN., STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO — 3d transition metal impurities in wide-gap oxides exist in multiple charged configurations[1], and may function as (i) donor/acceptor defects to modify carrier concentrations, (ii) magnetic elements to induce collective magnetism, and (iii) shift the host band edges. While previous investigations have addressed some of these phenomenologies separately, we link them together, and present the chemical trends for electronic properties, carrier doping, and magnetism along the series of 3d...3d8 impurities in the paradigmatic wide-gap oxide hosts ZnO and In2O3. For these general trends we find that, in In2O3 most 3d impurities are amphoteric and exhibit deep transitions, whereas in ZnO the early 3d impurities (Sc-V) have shallow donor transitions, and only the late 3d’s (Co, Ni, Cu) have acceptor transitions inside the band gap. Ferromagnetic interactions emerge upon the partial filling of 3d levels resonant inside the conduction band, an in general require electron doping from additional sources. [1] H. Raebiger, S. Lany, and A. Zunger, Nature 455, 783 (2008).

10:48AM H32.00013 Multifarious magnetism in copper oxide nanostructures from first-principles. X.-Y. CUI, A. SOON, University of Sydney, B. DELLEY, Paul Scherrer Institute, S.-H. WEI, National Renewable Energy Laboratory, C. STAMPFL, University of Sydney — Driven by the ever-increasing demand for novel spin-dependent advanced materials, investigation of nanoscale magnetic properties is currently actively pursued. With the latest developments focusing more on magnetic semiconducting oxides, materials based on cuprous oxide, Cu$_2$O, are of high interest as potential p-type semiconducting candidates. Thus developing an understanding of how intrinsic defects influence both its electronic and magnetic properties is important. We perform density-functional theory calculations to analyze both the electronic and magnetic properties of native defects in both bulk Cu$_2$O and its surfaces, as well as their respective formation/surface energies under different growth conditions. We find that under oxygen-lean conditions, the experimentally observed ferromagnetic behaviour [2] could originate from copper vacancies on Cu$_2$O(111) while under oxygen-rich conditions, low energy bulk oxygen interstitials might explain the ferromagnetic moment found in the same material. This suggests that the origin of observed magnetism in sub-stoichiometric copper oxide nanoparticles could be multifarious, highlighting the complimentary role of bulk and surface native magnetic defects.

8:00AM H33.00001 Observation of the Josephson effect in Pb/Ba$_{1-x}$K$_x$Fe$_2$As$_2$ single crystal junctions, XIAOHANG ZHANG, RICHARD GREENE, ICHIRO TAKEUCHI, University of Maryland, College Park, YOON SEOK OH, YONG LIU, LIQIN YAN, KEE HOON KIM, Seoul National University — We have fabricated Josephson junctions using single crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and Pb (or Pbln) as the counter electrode in two geometries. The c-plane single crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ were synthesized by the Sn-flux method with the nominal composition of $x = 0.4$. In one junction geometry, Ag (30 nm) and Pbln (200 nm) were evaporated on the surface of the crystals. In the other geometry, a Pb point contact was used. Both geometry junctions show resistively shunted junction $I-V$ curves below the $T_c$ of the counter electrode. Microwave induced steps were observed in the $I-V$ curves, and the critical currents are completely suppressible with applied magnetic field in a manner consistent with a small junction limit. $IcR_N$ products of up to 0.3 mV have been observed in these junctions at 4.2 K. The observation of Josephson coupling along the c-axis between an iron pnictide superconductor and a conventional superconductor suggests the existence of a non-d-wave superconducting order parameter in iron pnictide superconductors.

8:12AM H33.00002 ABSTRACT WITHDRAWN

8:24AM H33.00003 Multigap superconductivity in pnictides, PETER SAMUELY, PAVOL SZABO, ZUZANA PRIBULOVÁ, GABRIEL PRISTAS, Centre of Low Temperature Physics Kosice, PAUL CANFIELD, SERGEY BUD’KO, Ames laboratory, INSTITUTE OF EXPERIMENTAL PHYSICS, SLOVAK ACADEMY OF SCIENCES, 04001 KOSICE, SLOVAKIA TEAM, AMES LABORATORY AND IOWA STATE UNIVERSITY, AMES, IA 50011, USA TEAM — Point-contact Andreev reflection studies of the superconducting energy gap on the NdFeAsO$_x$(Ba,K)$_2$Fe$_2$As$_2$ and BaFe$_2$(Co$_{1-x}$V$_x$)$_2$As$_2$ crystals will be presented. The analysis of the data points to a two-gap superconductivity in these materials. Possible existence of the pseudogap in the non-superconducting density of states related to the static or dynamic magnetic order will be discussed as well.

8:36AM H33.00004 Coexistence of two order parameters and a pseudogap in the iron-based superconductors, RENATO GONNELLI, Dipartimento di Fisica and CNISM, Politecnico di Torino, Italy — The number, the symmetry and the amplitude of the order parameters (OPs) in the Fe-As superconductors are still open issues, as well as the origin of the electron pairing. To address these issues, we performed point-contact Andreev-reflection measurements in SmFeAsO$_x$F$_{2-x}$ ($T^{\text{crit}} = 53$ K) and LaFeAsO$_x$F$_{0.1}$ ($T^{\text{crit}} = 27$ K) polycrystals. In both cases, the low-temperature conductance curves clearly indicate the presence of two OPs in the superconducting state. No zero-bias peaks were observed, which — considering the non-directional current injection — clearly rules out the d-wave symmetry. If a superconducting character is supposed for both the OPs, their amplitudes can be extracted from a generalized two-band BTK fit (with two s-wave gaps, as in MgB$_2$) of the normalized conductance curves. The fit is indeed very good and gives OP amplitudes, $\Delta_1$ and $\Delta_2$, that lie slightly below and well above the BCS value, respectively. In Sm-1111, their low-temperature values are $\Delta_1(0) = 6.15 \pm 0.50$ meV and $\Delta_2(0) = 18 \pm 3$ meV, which give gap ratios (2$\Delta/K_BT_c$) of about 2.7 and 8.0. Both $\Delta_1$ and $\Delta_2$ show a BCS-like temperature dependence and close at the bulk $T_c$. In La-1111 we obtained point contacts with different local $T_c$s (from 27.3 to 31.0 K) in crystallites with slightly different doping. Here $\Delta_1$ shows a non-BCS temperature dependence with a high-temperature “tail,” while $\Delta_2$ seems to close at $T < T_c$. While the low-temperature gap $\Delta_1(0)$ increases on increasing $T_c$ (remaining always around the BCS value), $\Delta_2(0)$ decreases and finally disappears when $T_c = 31$ K, reminding the case of cuprates. At $T_c$, the normal-state conductance is asymmetric and shows features at zero bias (a depression or pseudogap in La-1111, a hump in Sm-1111) that however are also present in the superconducting state and are progressively washed out on increasing temperature, to finally disappear at $T_c \approx 140$ K, close to the Néel temperature of the parent compound.

9:12AM H33.00005 Point-contact Andreev reflection tunneling spectroscopic (PCARTS) study on Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, XIN LU, W. K. PARK, L. H. GREENE, Physics and FSMLR, UIUC, H. Q. YUAN, Zhejiang University, China, G. F. CHEN, G. L. LUO, N. L. WANG, Institute of Physics, CAS, Beijing, A. SEFAT, M. A. MCGUIRE, R. JIN, B. C. SALES, D. MANDRUS, MSTD, Oak Ridge National Lab. — PCARTS is applied to investigate the gap structure in the newly-discovered iron pnictide superconductors Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$. Double peaks due to Andreev reflection with strongly-sloping background are frequently observed in the conductance curves G (V) on the Au-Ba$_{1-x}$K$_x$Fe$_2$As$_2$ point-contact junctions on the freshly-cleaved surface along the c-axis. If normalized by the background baseline and analyzed by Blonder-Tinkham-Klapwijk model, the data show a gap size $\sim 4$ meV with $2\Delta/K_BT_c \sim 2.6$. However, it is observed that, for the Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, G (V) curves evolve from V-shape to zero-bias conductance peak with increasing tip pressure, where the tip is likely to penetrate through surface layer. The existence of surface oxide layer is confirmed by comparative XPS characterization on freshly-cleaned and uncleaned surfaces.

9:24AM H33.00006 ABSTRACT WITHDRAWN

9:36AM H33.00007 Probing the Spin-Density-Wave Transition in SmOFeAs using Point-Contact Spectroscopy, T. Y. CHEN, S.X. HUANG, JHU, R. H. LIU, X. H. CHEN, USTC, C. L. CHEN, JHU, JOHNS HOPKINS UNIVERSITY COLLABORATION, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA COLLABORATION — In spring 2008, a new family of superconductors with the general composition of SmFeAs(O$_{1-x}$F$_x$) has been discovered. The metallic parent compound SmFeAsF has a spin-density-wave (SDW) transition near 150 K with hysteretic temperature dependence in magnetic structure, crystalline structure, and resistance. Doping the parent compound with fluorine results in the suppression of the SDW transition and the emergence of superconductivity with transition temperatures up to 55 K. Some theories suggest that the SDW transition may be intimately related to the superconductivity. In this work, we use point-contact spectroscopy to investigate the SDW transition in the parent SmOFeAs compound. Instead of varying temperature, under a high bias voltage a small region underneath a point contact can be heated up through the SDW transition, resulting in differential conductance peaks. Similar to the temperature dependence of the resistance and structure, the SDW transition is hysteretic with bias voltage at the transition. We further show that this feature in differential conductance, which may be easily mistaken as a pseudo gap of a superconductor, is actually a characteristic of the ballistic heating effect.
Recent discovery of superconductivity in the iron based LaFeAsO\textsubscript{1-x}F\textsubscript{x} stimulation great interests as a new class of non-cuprate compound. We calculate the surface density of state of LaFeAsO\textsubscript{1-x}F\textsubscript{x} superconductor. The gap function is obtained microscopically by solving the Eliashberg equation in a 5-band Hubbard model with the random phase approximation (RPA). Green’s function of the surface state is obtained by inserting infinite potential barriers using Matsumoto and Shiba method. Although the gap function has a sign change between Fermi surfaces, we cannot find mid gap Andreev bound state in [100] and [110]-oriented interface.

Novel properties in Josephson junctions involving \( s_{\pi/2} \)-pairing state in Iron-Pnictides. WEI-FENG TSAI, DAO-XIN YAO, JIANGPING HU, Purdue University, B. ANDREI BERNEVIG, Princeton University — We present theoretical results of Andreev bound states in superconductor-normal metal (or insulator)-iron-pnictide junctions. Within the two-orbital exchange coupling model [1], the presence of non-trivial in-gap states, which uniquely appear in the theoretical results of Andreev bound states in superconductor-normal metal (or insulator)-iron-pnictide junctions. Within the two-orbital exchange coupling model [1], the presence of non-trivial in-gap states, which uniquely appear in the s-wave \( \cos k_x \cos k_y \) (\( s_{\pi/2} \)) pairing state, can be taken as a sharply distinct feature in contrast to other singlet pairing states. In addition, a proposed novel trilayer \( \pi \)-junction involving \( s_{\pi/2} \) superconductivity is also discussed as a new possible signature of such unconventional pairing symmetry.

Possible phase-sensitive test of pairing symmetry in superconducting pnictides, DAVID PARKER, IGOR MAZIN, U.S. Naval Research Laboratory — The discovery of the new class of pnictide superconductors has engendered a controversy about their pairing symmetry, with proposals ranging from an extended \( s \)-wave or “\( s_{\pi} \)” symmetry to nodal or nodeless d-wave symmetry to still more exotic order parameters such as p-wave. Although there is evidence that a fully gapped state may exist in the pnictides, the symmetry of this state remains indeterminate. Building on the earlier, similar work performed for the cuprates, we propose here a phase-sensitive Josephson interferometry experiment that may allow resolution of the issue, taking into consideration novel features such as the local orbital character (from DFT calculations), and employing a particular potential barrier to restrict the tunneling orientations to favorable directions.

Andreev Bound states as a phase sensitive probe of the pairing symmetry of the FeAs superconductors, POUYAN GAHEMI, UC Berkeley, FA WANG, ASHVIN VISHWANATH, UC Berkeley & LBNL — A leading contender for the pairing symmetry in the Fe-As-pnictide high temperature superconductors is extended \( s \)-wave \( s_{\pi} \), a nodeless state in which the pairing changes sign between Fermi surfaces. Verifying such a pairing symmetry requires a special probe that is sensitive to both phase and magnitude of the order parameter. We show that the sign structure of \( s_{\pi} \) pairing leads to Andreev bound states at the edge. In the clean limit they only occur when the edge is along the Fe-Fe bond, but not for a diagonal edge. In contrast to d-wave Andreev bound states, they are not at zero energy and, in general, do not produce a zero bias tunneling peak. Consequences for tunneling measurements are derived, within a simplified two band model and also for a more realistic five band model.

Examining SrFe\textsubscript{2}As\textsubscript{2} with a Low Temperature Scanning Tunneling Microscope, FRANCIS NIESTEMSKI, Boston College Dept. of Physics, J. GILLET , SUCHITRA SÉBASTIAN, Cavendish Laboratory, University of Cambridge, VIDYA MADHAVAN, Boston College Dept. of Physics — The new pnictide superconductors have generated huge excitement. These materials are the first to add some chemical diversity to the limited high-Tc list previously exclusive to cuprates. We examine the pnictide material parent compound SrFe\textsubscript{2}As\textsubscript{2} with a low-temperature ultra-high vacuum scanning tunneling microscope (STM) at 4 K. We find multiple types of topography and spectroscopy with low energy features. We relate our data to results from ARPES and other experiments.

Electronic Structure on (001) Surface of Co-doped BaFe\textsubscript{2}As\textsubscript{2} Studied with Scanning Tunneling Spectroscopy\(^1\). A. LI, D. R. JAYASUNDARA, Y. XIUAN, J. P. O’NEAL, Y. CHEN, W. KIM, C. S. TING, S. H. PAN, University of Houston, Houston, Texas 77204-5002, R. JIN, E. W. PLUMMMER, Louisiana State University, Baton Rouge, LA 70803-4001, R. JIN, A. S. SEFAT, M. A. MCGUIRE, B. C. SALES, D. MANDRUS, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Co-doping makes the pnictide compound BaFe\textsubscript{2}As\textsubscript{2} superconducting. We cleave the single crystals of this compound in UHV and study their surfaces with a low temperature STM. In this talk, we present the scanning tunneling spectrum obtained on the (001) surface of the optimally doped BaFe\textsubscript{2}As\textsubscript{2} single crystals (Tc = 23K) and compare these spectra with the ones obtained on the surface of the parent compound. We have found that the major feature of the spectra on the superconducting compounds is the opening of a superconducting gap of about 6 meV for the optimally doped one. We have also observed other detailed spectrum features. We will discuss the relation between spectrum features and the local environment and also present some theoretical fit to the superconducting energy gap spectrum.

\(^1\)Funding support from Texas Center for Superconductivity at UH, Robert A. Welch Foundation, and from DOE-BES-DMSE

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8:00AM H34.00001 Resistivity and superfluid density measurements on under- and over-doped La\textsubscript{2-x}Sr\textsubscript{x}CuO\textsubscript{4} films. THOMAS LEMBERGER, IULIAN HETEL, The Ohio State University, A. TSUKADA, MICHIO NAITO, Tokyo University of Agriculture and Technology — We have measured the resistivities and superfluid densities (or, penetration depths, \( \lambda \)) of a series of LSCO films with a wide range of Sr concentrations. Films are grown by MBE on LaSrAlO\textsubscript{4} substrates under nominally identical conditions. Due to substrate mismatch, films are under compression, Resistivities decrease smoothly as Sr concentration increases, and resistive transitions are sharp. Tc has a maximum at \( x \approx 0.18 \). Interesting features in the T-dependence of \( 1/\lambda^2 \) will be discussed. Absolute values of resistivity and superfluid density in these films indicates quality comparable to bulk materials. Falloff of superfluid density with overdoping, together with a smooth decrease in resistivity, is consistent with an interpretation in terms of a mesoscopically inhomogeneous superconducting state.
8:12AM H34.00002 Strong Reduction of Tc, Suppression by Magnetic Field in YBa2Cu3O7−x Films with Dispersed Nanoparticles, E. Cimpoiasu, J. D. Feldmann, U. S. Naval Academy, C. V. Varanasi, T. J. Haugan, P. N. Barnes, G. A. Levin, Air Force Research Laboratory — Improvements in the critical current density Jc in applied magnetic fields are of great importance for applications of the YBa2Cu3O7−x coated conductors. Nanopulse inclusions have shown to be effective in increasing Jc, but the precise physical mechanisms of their action are elusive. A broader range of experiments is needed in order to elucidate the physics of this phenomenon. Here we discuss the magnetic field H- and temperature T-dependence of the resistivity of thin films in the normal state and near Tc. Pure YBCO films will be compared with those that contain either dispersed Y2O3/nanoparticles or Ba5Sn2O10 nanorods. The resistance of highly c-axis oriented YBCO films was measured by the Montgomery method in the range 20 K < T < 300 K and in fields up to 9 T. The films with inclusions show a much sharper and less broadened in-field transition (smaller Tc suppression by field) than pure YBCO. This correlates well with increased Jc measured by conventional methods and indicates increased pinning strength at all temperatures. In order to further identify the signatures of the nano-inclusions, the samples were annealed in air at 420 deg C. The changes induced by the annealing will be discussed. This work was partially supported by AFOSR and the AFRL Propulsion Directorate.

8:24AM H34.00003 Quantum Oscillations and Hall Resistivity in YBCO and Tl-2201: Exploring the Fermi Surface of the Cuprates, Brad Ramshaw, Univ British Columbia — The field of high temperature superconductivity has enjoyed something of a Renaissance in the past two years with the discovery of quantum oscillations in Shubnikov de Haas and de Haas-van Alphen measurements preformed on YBCO and Tl-2201. DC transport measurements around the one eighth hole doping region of high Tc phase diagram have shown a temperature and doping dependence to the Hall coefficient. In this doping region the Hall coefficient changes sign from positive to negative as temperature goes to zero, indicating a competition of mobilities between holes and electrons. In high magnetic fields these measurements also exhibit oscillations in one over the field strength, indicating the existence of small pockets of Fermi surface. This information, coupled with the Hall data, gives rise to the interpretation that the large hole like Fermi surface found in the overdoped region on Tl-2201 reconstructs into smaller electron like Fermi pockets on the underdoped side. Combined with other theoretical and experimental techniques, these experiments are allowing us to develop an understanding of the electronic structure of the cuprates across the entire phase diagram. This understanding is crucial to uncovering the underlying mechanism that gives rise to high temperature superconductivity.

8:36AM H34.00004 Longitudinal and Transverse Transport properties of disordered graphene, Vincent Ugarte, Vivek All, Department of Physics and Astronomy, University of California-Riverside, California 92521, USA — We present results of calculations of the properties of thermal and electrical transport coefficients of disordered graphene in a weak magnetic field. In particular, we are interested in the vanishing of density of states and units and scattering on transport coefficients near the Dirac point. The effect of impurity states is included within a self-consistent t-matrix approximation. We find a peak in both the Nernst coefficient and thermopower around the chemical potential which grows as one approaches the Dirac point. Our experiments are a rich source of data to test the theories and models that have been developed to describe transport through disordered graphene.

8:48AM H34.00005 Linear-T resistivity and change in Fermi surface at the pseudogap critical point of a high-Tc, superconductor, Ramzy Daou, Nicolas Doiron-LeRaud, David Leboeuf, Shiyang Li, Francis Laliberte, Olivier Lour-Choineire, Universite de Sherbrooke, J.Y. Jo, Luis Balicas, NHMFL Tallahassee, J.-Y. Qian, J.-S. Zhou, John Goodenough, Texas Materials Institute, Universite de Sherbrooke and Canadian Institute for Advanced Research — A fundamental question of high-temperature superconductors is the nature of the pseudogap phase which lies between the Mott insulator at zero doping and the Fermi liquid at high doping. Here we report on the behaviour of charge carriers near the zero-temperature onset of that phase, namely at the critical doping p* where the pseudogap temperature Tg goes to zero, accessed by investigating a material in which superconductivity can be fully suppressed by a steady magnetic field. Just below p*, the normal-state resistivity and Hall coefficient of La2−xNd2−xSrxCuO4 are found to rise simultaneously as the temperature drops below Tg, revealing a change in the Fermi surface with a large associated drop in conductivity. At p*, the resistivity shows a linear temperature dependence as T → 0, a typical signature of a quantum critical point. These findings impose new constraints on the mechanisms responsible for inelastic scattering and Fermi-surface transformation in theories of the pseudogap phase.

9:00AM H34.00006 Transport Properties in Electron-Doped La2−xCexCuO4 Thin Films, Kui Jia, Xiaohang Zhang, Paul Bach, Richard Greene, University of Maryland, College Park — The electron-doped high-Tc cuprate La2−xCexCuO4 (LCCO) is quite different from other members, such as Pr2−xCe3−xO7, CeO2, and BaSrCuO3. One distinct difference is that the optimal Ce doping in LCCO is ~0.10, compared to ~0.15 in PCCO and NCBO. Here, we will present a detailed and systematic study of the magnetic field and temperature dependence of the transport properties of LCCO, including the low-temperature Hall effect and in-plane angular magnetoresistance.

1This work was supported by NSF-DMR 0653535.

9:12AM H34.00007 Evidence for individual quantum phase-slip events in homogeneous superconducting nanowires, Mitrabanu Sahai, Myung-Ho Bae, University of Illinois at Urbana-Champaign, Andreuy Rogachev, University of Utah, David Pekker, Harvard University, Nayana Shah, University of Illinois at Urbana-Champaign, Tzu-Chieh Wei, University of Waterloo, Paul Goldbart, Aleksey Bezryadin, University of Illinois at Urbana-Champaign — We report strong evidence for individual quantum tunneling events undergone by the superconducting order-parameter field in homogeneous Mo2Te2Sb nanowires. We obtain this via measurements of the distribution of switching currents, whose width exhibits a rather counter-intuitive, monotonic increase with decreasing temperature. We outline a stochastic model of phase-slip kinetics, which relates the basic phase-slip rates to switching rates. Comparison with this model indicates that the phase predominantly slips via thermal activation at high temperatures, but at sufficiently low temperatures switching is caused by individual topological tunneling events of the order-parameter field, i.e., quantum phase slips (QPS). Importantly, measurements on several wires show that quantum fluctuations tend to dominate over thermal fluctuations at larger temperatures in wires having larger critical currents. This fact supports the view that the anomalously high switching-rates observed at low temperatures are indeed due to QPS, and are not consequences of extraneous noise or inhomogeneity of the wire.

9:24AM H34.00008 Collapse of peak effect by alternating current and its frequency dependence in MgCNi3 single crystal, Dong-Jin Jang, Department of Physics, Pohang University of Science and Technology, Pohang, 790-784, Republic of Korea, Hyun-Sook Lee, Department of Physics, Pohang University of Science and Technology, Pohang, 790-784, Republic of Korea, H-G Lee, National Creative Research Initiative Center for Superconductivity and Department of Physics, Sogang University, Seoul 121-742, Republic of Korea — The peak effect, which appears as sharp rise in critical current near superconductor-normal transition of a superconductor, is first order phase transition. However, if vortices happen to move across sample by direct current (DC), sharp transition nature becomes blunted by edge contamination as intensively studied in NbSe2. This edge contamination has been shown to be removed by alternating current (AC) or by using edgeless Corbino geometry. Among few superconducting materials showing peak effect, MgCNi3 exhibits fairly sharp peak effect even in DC strip geometry. And remarkably, critical current measured by using AC is greatly suppressed as frequency of AC increases.
9:36AM H34.00009 Analytical Procedure for Measuring Electrical Resistivity of Anisotropic Materials, C.A.M. DOS SANTOS, B.S. DE LIMA, C.Y. SHIGUE, Escola de Engenharia de Lorena - USP, Lorena-SP, Brazil, A. DE CAMPOS, M.S. DA LUZ, A.T. RICE, B.D. WHITE, J.J. NEUMEIER, Department of Physics - MSU, Bozeman-MT, USA — The Montgomery method is used to determine the resistivity tensor of anisotropic materials [1] such as high-T_c and FeAs superconductors, 2-layer Mn oxides, organic conductors, and quasi-1D conductors. It uses the Wasscher transformation [2], which calculates an isotropic equivalent sample of the anisotropic sample. This is a timing-consuming task because it is a numerical method based upon graphical analyses obtained from calculations by Logan, Rice, and Wick [3]. In this work we report a simplification of the Montgomery method. Analytical equations are derived and applied to several isotropic and anisotropic samples (Cu, Al, Bi_{2}Sr_{2}CaCu_{2}O_{8+d}, Graphite, SnN_{2}O_{5}, \gamma-Mo_{2}O_{3}). Comparisons with results obtained using the standard four-probe method demonstrate the quality and simplicity of the procedure, which can easily be extended to data acquisition systems. This material is based upon work supported by FAPESP (grant No. 07-04572-8), NSF (grants Nos. DMR-0504769 and 0552458), and CNPq (grant Nos. 301334/2007-2 and 201439/2007-7). [1] H. C. Montgomery, J. Appl. Phys. 42, 2971 (1971). [2] J. D. Wasscher, Philips Res. Repts. 16, 301 (1961). [3] B. F. Logan, S. O. Rice, and R. F. Wick, J. Appl. Phys. 42, 2975 (1971).

9:48AM H34.00010 Doping dependence of the dynamic and static critical exponents in Pr_{2-x}Ce_{x}CoO_{4}, M.C. SULLIVAN, R. ISAACS, J.B. OLSON, J. SOUSA, M. SALVAGGIO, Department of Physics, Ithaca College, Ithaca NY, R.L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — Scaling analysis of voltage vs. current isothersms is a favorite tool to study the normal-superconducting phase transition in cuprate superconductors. This measurement has never been performed on the electron-doped cuprate superconductor Pr_{2-x}Ce_{x}CoO_{4}, due in part to difficulties which result from finite-thickness effects, even in thick (d \approx 3000\AA) films [2]. If finite-thickness effects are taken into consideration, we can find the critical isotherm and the dynamic critical exponent, and we can use small magnetic fields to find the static critical exponent. Similar measurements have been made on the more familiar hole-doped cuprates such as YBa_{2}Cu_{3}O_{7} [3]. We present our results of the dynamic critical scaling exponent z and static critical exponent \nu in our Pr_{2-x}Ce_{x}CoO_{4} films as a function of doping.

10:00AM H34.00011 Experimental study of superconductivity in single crystal few-layer NbSe_{2} and the effect of high electric fields, NEAL STALEY, Pennsylvania State University, LIJUN LI, ZHUAN XU, Zhejiang University, China — We report many studies on superconducting properties in two dimensional films. However, a detailed study of superconducting properties in the two-dimensional limit when crystallinity is still retained, which will allow the probing of band dependent superconductivity in 2D, has not been performed. Due to concerns over defects in ultra thin films deposited in the usual methods, we use the methods developed in preparing micromechanically exfoliated graphene devices. In these samples the band structure is present while maintaining extremely low defect density. Inspired by this simple process that created single crystal single sheet graphene we fabricated ultra thin single crystalline NbSe_{2} flakes ranging from single to many sheets as estimated using an optical technique correlated to AFM and Raman spectroscopy measurements. Transport and planar tunnel junction devices were fabricated using standard ebeam lithography techniques. We will also study the behavior of of these devices in high electric fields.

10:12AM H34.00012 Size effects in the nonlinear resistance in a virtual Berezinskii-Kosterlitz-Thouless state of superconducting films, ALEX GUREVICH, National High Magnetic Field Laboratory, VALERII VINOKUR, Argonne National Laboratory — We show that the size effects strongly affect the nonlinear electric field-current (E, A) relation of superconducting films. We calculate E(J) due to thermally-activated hopping of single vortices driven by current J across the film in a magnetic field H, taking into account interaction of free vortices with their antivortex images and peaks in the Meissner currents at the film edges. Unbinding of virtual vortex-antivortex pairs not only mimics the transport uniform BKT behavior, it can dominate the observed E(J) and result in the field-dependent ohmic resistance at small J. We show that E(J) can be tuned by changing the film geometry and propose experimental tests of this theory.

10:24AM H34.00013 Geometric Effects on the Tunneling Apparent Barrier Height, ARAN GARCIA-LEKUE, THOMAS FREDERIKSEN, DIPC, Donostia International Physics Center, ANDRES ARNAU, Centro de Fisica de Material — An experimental quantity which may help understanding the mechanism of electron tunneling, in STM experiments or across broken nanojunctions for example, is the apparent barrier height. In order to extract information from this experimental observable one can consider a simple one-dimensional tunneling model, where the apparent barrier height is the rate of change of the logarithm of the conductance with the tip-apex separation or vacuum gap. Theoretically, a faithful analysis of the apparent barrier height requires a precise description of the tunneling conductance in the vacuum region. However, most of the conductance calculations are performed using atom centered localized basis sets, which cannot adequately describe the tunneling current crossing the vacuum gap and can therefore lead to erroneous results. In this work, we present tunneling conductance calculations obtained using the transport calculation method introduced in Ref. [1]. Since this method employs a plane-wave basis set, it provides accurate results for the electron tunneling across the vacuum gap and, consequently, for the apparent barrier height. Here, we report results for broken Au nanojunctions with different geometries, which allows us to thoroughly investigate geometric effects on the apparent barrier height. 1. A. Garcia-Lekue and L.W. Wang, Phys. Rev. B 74, 245404 (2006).

10:36AM H34.00014 Thermopower across the pseudogap critical point of La(1.6-x)Nd(0.4)Sr(x)CuO(4): Evidence for a quantum critical point in a hole-doped high-Tc superconductor, OLIVIER CYR-CHIOINERE, RMZI DAOU, FRANCIS LALIBERTÉ, DAVID LEBEUFF, NICOLAS DOIRON-LEYRAUD, Université de Sherbrooke, JIAQIANG YAN, JIANSHI ZHOU, JOHN B. GOODENOUGH, Texas Material Institute, U of Texas at Austin, LOUIS TAILLEFER, Universite de Sherbrooke — The thermopower S of the high-Tc superconductor La(1.6-x)Nd(0.4)Sr(x)CuO(4) was measured as a function of temperature T near its pseudogap critical point, the critical hole doping p^* where the pseudogap temperature T^* goes to zero. Just above p^*, S/T varies as ln(1/T) over a decade of temperature. Below p^*, S/T undergoes a large increase below T^*. As with the temperature dependence of the resistivity, which is linear just above p^* and undergoes a large upturn below T^*, these are typical signatures of a quantum phase transition. This suggests that p^* is a quantum critical point below which some order sets in, causing a reconstruction of the Fermi surface, whose fluctuations are presumably responsible for the linear-T resistivity and logarithmic thermopower. We discuss the possibility that this order is the "stripe" order known to exist in this material.

10:48AM H34.00015 Low-Temperature Thermal Conductivity in a d-Wave Superconductor with Coexisting Checkerboard Charge Order, PHILIP SCHIFF, ADAM DURST, Stony Brook University — Given the experimental evidence of charge order in the underdoped cuprate superconductors, we consider the effect of coexisting checkerboard charge order on low-temperature thermal transport in a d-wave superconductor. We compute the quasiparticle excitation spectrum in the presence of both order parameters and perform a diagrammatic Kubo formula calculation of the zero-temperature thermal conductivity tensor as a function of the magnitude and wave vector of the charge order. Results depend on disorder, indicating that, in the presence of charge order, zero-temperature thermal transport is no longer universal.
8:00AM H35.00001 Effects of Magnetic Order and Pairing on the Fermi Surface of the Pnictides¹ . A. MOREO, M. DAGHOFER, R. YU, Oak Ridge National Lab, University of Tennessee, J. A. RIERA, Universidad Nacional de Rosario, Argentina, E. R. DAGOTTO, Oak Ridge National Lab, University of Tennessee — Based on numerical and mean-field calculations performed on models for the FeAs planes of the newly discovered Fe-based superconductors, we present results for the expected shape of the Fermi surface both in the undoped and the doped regime. In the undoped case, numerical studies, Lanczos and VCA, are performed for a two-orbital model, while a mean-field formalism allows us to study a more realistic 4 orbital case. A pocket structure is obtained for the intermediate Hubbard coupling regime of parameters in which the system is magnetically ordered but still metallic.[1] We construct a mean-field model for light electronic doping based on the pairing operator that is found by the unbiased Lanczos calculations in the two orbital model, i.e. a spin singlet, orbital even, operator transforming according to the $B_{2g}$ representation of the group $D_{4h}$. [2] We present the resulting nodal structure [3] and discuss comparisons with ARPES results.

1Supported by the NSF grant DMR-0706020, the Div. of Materials Sciences and Eng., U.S. DOE under contract with UT-Batelle, LLC

8:12AM H35.00002 Nematic spin order and spin-lattice coupling in Fe-based Superconductors , JIANGPING HU, CHEN FANG, WEI-FENG TSAI, Purdue University, HONG YAO, STEVE KIVELSON, Stanford University — We show that the structure transitions observed in Fe-based superconductors are magnetically driven. A quantum Heisenberg model ($J_{1} - J_{2} - J_{3}$) exhibits a sequence of two phase transitions: from a high temperature symmetric phase to a narrow region of intermediate “nematic” phase, and then to a low temperature spin ordered phase when $J_{2}$ is small. Identifying phases by their broken symmetries, these phases correspond precisely to the sequence of structural (tetragonal to monoclinic) and magnetic transitions that have been recently revealed in neutron scattering studies of 1111 series of Fe-based superconductors. The structural transition can thus be identified with the existence of incipient (“fluctuating”) magnetic order. We also discuss the effect of spin-lattice coupling on the phase diagram of the model.

Reference: Chen Fang, Hong Yao, Wei-Feng Tsai, JiangPing Hu and Steven A. Kivelson, Phys. Rev. B 77 224509 (2008).

8:24AM H35.00003 Modeling of Fe pnictides: the Magnetic Order and Pairing Channels¹ . M. DAGHOFER, A. MOREO, Oak Ridge National Lab, University of Tennessee, J. A. RIERA, Universidad Nacional de Rosario, Argentina, E. ARRIGONI, TU Graz, Austria, D. J. SCALAPINO, University of California, Santa Barbara, E. R. DAGOTTO, Oak Ridge National Lab, University of Tennessee — We use numerical methods - exact diagonalization and the variational cluster approach - to study a two-orbital model for Fe-pnictide superconductors, including onsite Coulomb interaction $U$ and Hund’s rule coupling $J$.[1] Robust next-nearest neighbor hoppings stabilize the spin “striped” AF order for undoped clusters, in agreement with neutron scattering data. The ordered magnetic moment depends on $U$ and $J$, and we find a bad metal with small ordered moment at intermediate $U$, as observed experimentally. By adding two electrons to the undoped cluster, we identify three different pairings channels: An inter-orbital triplet at small $U$, which transforms as the $A_{1g}$ representation of the $D_{4h}$ group, an inter-orbital singlet transforming as $B_{2g}$ at the most realistic intermediate $U$, and an intra-orbital $A_{1g}$ singlet at large $U$. We compare the results to a three-orbital model including the $xy$ orbital in addition to the $xz$ ans $yz$ orbitals. [1] M. Daghofer et al., arXiv:0805.0148, to appear in PRL.

1Support from the NSF grant DMR-0706020; U.S. DOE under contract with UT-Batelle, LLC; Austrian Science Fund grant P18551-N16

8:36AM H35.00004 Existence of a metallic magnetically ordered state at intermediate Hubbard couplings in multi-orbital models for undoped iron pnictides¹ , RONG YU, University of Tennessee and ORNL, KIEN TRINH, University of Southern California, ADRIANA MOREO, MARIA DAGHOFER, University of Tennessee and ORNL, JOSE RIERA, Universidad Nacional de Rosario, Argentina, STEPHAN HAAS, University of Southern California, ELBIO DAGOTTO, University of Tennessee and ORNL — We present the results of a mean-field study for models that describe undoped iron pnictides. A realistic four-orbital model including iron orbitals in addition to the $d_{xz}$ and $d_{yz}$ orbitals is mainly discussed. Results for a two-orbital model with $d_{xz}$ and $d_{yz}$ orbitals are also shown. In both models, we report the existence of a novel intermediate coupling regime where the system is metallic and exhibits a striped spin order. Several properties of this state are discussed. By performing a mean-field study of other models for iron pnictides, we argue that such a metallic striped ordered phase is a general feature of the theoretical models describing iron pnictides.[1]

1This work was mainly supported by the NSF grant DMR-0706020 and the Division of Materials Science and Engineering, U.S. DOE, under contract with UT-Battelle, LLC.

8:48AM H35.00005 Low Ordered Magnetic Moment in Fe-As High-Tc Superconductors by Violation of Hund’s Rule¹ , JOSE RODRIGUEZ, California State University at Los Angeles, EDWARD REZAYI, California State University at Los Angeles — We study by exact diagonalization the $J_{0}$-$J_{1}$-$J_{2}$ model over the square lattice that Si and Abrahams introduced recently to describe magnetism in the newly discovered iron-arsenic class of high-Tc superconductors. The case of maximum frustration between the nearest-neighbor and the next-nearest-neighbor Heisenberg exchange terms, $J_{2} = \frac{1}{2}J_{1}$, over a 4 by 4 square lattice with periodic boundary conditions is focused on. Each site hosts two Fe orbitals. Hidden long-range antiferromagnetic order can appear in the absence of Hund’s rule coupling, $J_{0} = 0$. It shows no net ordered magnetic moment. The ordered collinear/SDW moment steadily increases from zero as Hund’s rule coupling turns on: $J_{0} < 0$. This result compares well with recent determinations of a low ordered magnetic moment for the insulating parent compounds of Fe-As based high-Tc superconductors by elastic neutron scattering. Our numerical results are also consistent with a quantum phase transition at intermediate Hund’s rule coupling, $J_{0} = -2|J_{1}|$, that separates the latter hidden-order state from a more familiar frustrated magnetic state that obeys Hund’s rule.

1Research supported in part by the Air Force Office of Scientific Research under grant no. FA9550-06-1-0479
9:00 AM H35.00006 Magnetic Excitations in the Iron-based Superconductors1. DAOXIN YAO, JIANPING HU, ERICA W. CARLSON, Department of Physics, Purdue University — We calculate the expected inelastic neutron scattering response based on the spin-orderings found in the iron-based superconductors, using spin-wave theory. For the two-sublattice collinear antiferromagnet, we consider two types of superexchange couplings between Fe atoms: nearest-neighbor coupling $J_1$ and next-nearest-neighbor coupling $J_2$. We show how to distinguish experimentally between ferromagnetic and antiferromagnetic $J_1$. We show the existence of saddlepoints near ($\pi$, $\pi/2$) and (0, $\pi/2$), which are expected to give rise to extra scattering intensity. We find that the sublattice magnetization can be reduced by the zero-point motion of spin waves, although not enough to account for the small moments observed in experiment. By comparison with experimental results on SrFeAs$_2$, we estimate that the effective magnetic interlayer coupling is rather large, about 1/8 the value of the in-plane couplings. References: 1) Phys. Rev. Lett. 101, 167203 (2008); 2) Phys. Rev. B 78, 052507 (2008)

1DXY is supported by NSF DMR-0804748, JPH is supported by NSF PHY-0603759 and E. W. C. is supported by Research Corporation.

9:12 AM H35.00007 Iron pnictides as a model system for heavy fermion behavior: influence of conduction-electron magnetic ordering on Kondo effect. JIANHUI DAI, Zhejiang University, QIMIAO SI, Rice University, JIAN-XIN ZHU, LANL. — The rare-earth iron pnictides exhibit a number of magnetic ground states besides the unconventional superconductivity. With CeOfEP [1] and CeOfEAs [2] in mind as prototypes, we develop an extended Anderson lattice model which incorporates the hybridizations of the 5p (4p or 3p)-orbitals with both the iron 3d-orbitals and rare earth 4f-orbitals[3]. We show a new type of Kondo lattice physics: Kondo screening of the f-moments are suppressed by the antiferromagnetic ordering of the d-electrons. Inside the d-electron AF state (as in CeOfEAs), the f-moments are dominantly coupled by superexchange with competing components. The resulting magnetic frustration in general favors a helical order. The regime where d-electrons are paramagnetic (including CeOfEP) features the usual RKKY vs. Kondo competition. The implications of our results for heavy fermion physics in general are discussed.


9:24 AM H35.00008 Tight-binding Hamiltonian for LaFeAsO. DIMITRIOS PAPACONSTANTOPoulos, LANE NIXON, George Mason University, MICHAEL MEHL, Naval Research Laboratory — There have been several first-principles calculations reported recently for the superconducting pnictide LaFeAsO and related compounds. In addition, tight-binding(TB) Hamiltonians for these systems have been constructed with varying degrees of success. In this work we have used the NRL-TB method to fit our LAPW results to a TB basis with the aim of reproducing the band structure very accurately. We have included the s and d orbitals of Fe, the s and p orbitals of As, and the p orbitals of O. We present a study of these TB results in terms of the effect of each of the above orbitals on how accurately the first-principles band structure can be reproduced. Finally, we assess the feasibility of carrying out many-body theory with a Hamiltonian that may contain more than just the d-Fe orbitals.

9:36 AM H35.00009 Competing magnetism and superconductivity in two-band metals. ANTON VORONTSOV, MAXIM VAVILOV, ANDREY CHUBUKOV, University of Wisconsin - Madison — Recently discovered FeAs-based superconductors have a distinct multiple band structure - the hallmark model for these metals, with one electronic and one hole band. Within this model, we treat on equal footing magnetic spin density wave (SDW) and superconducting (SC) orders. We find that at low doping, magnetism wins, but at higher dopings superconducting instability comes first. We discuss the type of a transition between the two states, incommensurate SDW order at finite dopings, and co-existence of SDW and SC orders at $T = 0$ and finite temperatures. Our results reasonably well explain the phase diagram of LaO$_{1-x}$Fe$_{1-x}$As compounds.

9:48 AM H35.00010 Superconductivity in the multiband matrix t-J1-J2 model and its implications for the iron pnictides. QIMIAO SI, PALLAB Goswami, PREDRAG NIKOLIC, Rice University, ELIHU ABRAMHS, Rutgers University — We describe the iron pnictides in terms of an incipient Mott picture. We use local moments with frustrating J1-J2 interactions to model the incoherent electronic excitations, and couple them to the coherent electronic carriers. The resulting multiband matrix t-J1-J2 model is analyzed in terms of a slave boson theory, leading to a superconducting phase diagram as a function of doping and J2/J1 ratio. The different pairing symmetries reflect a competition between the strong coupling effects of the J1-J2 interactions, and the kinematic effects associated with the multiple sheets of Fermi surfaces.

10:00 AM H35.00011 Electronic states and material dependences of Fe-based superconductors. MICHIYASU MORI, IMR, Tohoku Univ., TAKAMI TOHYAMA, Kyoto Univ., NAVID AFZAL SHOOSHARY, SADAMICHI MAEKAWA, Tohoku Univ. — In this study, we discuss the electronic states of Fe-based superconductors and its material dependences, in particular, by taking account of the bond angle dependences. First, we calculate the crystal field splitting (\Delta) of Fe 3d orbital coordinated by four As's. Next, the hopping integrals (t) are estimated by using the Slater and Koster fs method. Note that these parameters, t and $\Delta$, change with $\alpha$. Finally, we can obtain the dispersion relation as a function of $\alpha$. It is found that the spectral weights near the Fermi energy are dominated by yz, xz and x^2-y^2 orbitals. The yz and xz orbitals are higher in energy around the regular tetragonal geometry, in which $\alpha$ is almost 109°. On the other hand, those two orbitals become lower in energy for the larger value of $\alpha$. Such an orbital crossing is crucial for the electronic states. The ground state phase diagram is obtained by the Hartree-Fock calculation of multi-band Hubbard model.
Begtrup et al, Phys. Rev. Lett. 408
Yao et al, Phys. Rev. Lett., transmission electron micrographs of the same nanotube. Our current progress toward quantitative pyrometry will be described.

Electrical current. Diffraction-limited optical microscopy identifies the nanotube position and orientation, and allows direct comparison with high-resolution eye, using individual carbon nanotubes as filaments. A nanotube is suspended over a hole in a solid silicon substrate, and is heated to incandescence with the angle between the axes of the nanotubes on the thermal conductivity.

Extended two dimensional structures (papers) containing these junctions. The investigation includes the effects of chirality, the off set in atomic register and nanopapers. Equilibrium and non-equilibrium molecular dynamics simulations are performed on non-bonded and bonded (fused) nanotube junctions and have great potential as electronic thermal management materials. Here we present our theoretical investigations on thermal properties of nanotube junctions

Nanotube Nanopapers

1

The Wiedemann-Franz law is restricted to each branch with its specific temperature; (b) thermoelectric power vanishes due to electron-hole symmetry. The model depicts different regimes such as ballistic and diffusive and shows excellent agreement with diffusive carrier transport in 1D conductors.

(a) The Wiedemann-Franz law is restricted to each branch with its specific temperature; (b) thermoelectric power vanishes due to electron-hole symmetry. The modell depicts different regimes such as ballistic and diffusive and shows excellent agreement with diffusive carrier transport in 1D conductors.

Tuesday, March 17, 2009 8:00AM - 11:00AM –
Session H36 DCMP: Carbon Nanotubes: Electrothermal Transport and Raman Spectroscopy

8:00AM H36.00001 Restricted Wiedemann-Franz law in 1D conductors, MARCELO KURODA, Dept. of Physics and Beckman Institute, University of Illinois at Urbana-Champaign, JEAN-PIERRE LEBURTON, Dept. of Electrical and Computer Engineering and Beckman Institute, University of Illinois at Urbana-Champaign — We show that under external electric fields or thermal gradients, carrier distributions in one-dimensional (1D) conductors with linear E-k dispersion have different temperatures for forward and backward (branch) carrier populations, as a consequence of self-consistent carrier-heat transport. We derive the moment equations of the Boltzmann transport equation, in the presence of elastic scattering, for which: (a) The Wiedemann-Franz law is restricted to each branch with its specific temperature; (b) thermoelectric power vanishes due to electron-hole symmetry. The model depicts different regimes such as ballistic and diffusive and shows excellent agreement with diffusive carrier transport in 1D conductors.

8:12AM H36.00002 Observation of Joule heating in multi-walled carbon nanotubes by electron thermal Microscopy, KAMAL BALOCH, TODD BRINTLINGER, NORVIK VOSKIANIAN, JOHN CUMINGS, University of Maryland — We report Joule heating in multi-walled carbon nanotubes under voltage bias by using an electron thermal imaging technique [1]. Briefly, the temperature profile is obtained by observing the solid to liquid phase transitions of indium islands sub-100nm in diameter, thermally deposited on the back side of an electron transparent dielectric membrane. The high spatial-resolution maps thus obtained demonstrate that in the high-voltage-bias regime the thermal dissipation occurs not at the electrode contacts but along the entire length of the nanotube as predicted in [2]. The low temperatures involved (<200 C) extend previous results [3] into a new temperature regime. The implications of these results when combined with other observations in the literature will be discussed.


1(supported by the ACS Petroleum Research Fund)

8:36AM H36.00004 Thermal Transport Through Carbon Nanotube Junctions and Carbon Nanotube Nanopapers, CHARLES A. BARR, ALPER BULDUM, Department of Physics, The University of Akron — Carbon nanotubes have demonstrated exceptional thermal transport properties that show promise in a wide range of applications. Nanotube nanocomposites and nanopapers have great potential as electronic thermal management materials. Here we present our theoretical investigations on thermal properties of nanotube junctions and nanopapers. Equilibrium and non-equilibrium molecular dynamics simulations are performed on non-bonded and bonded (fused) nanotube junctions and extended two dimensional structures (papers) containing these junctions. The investigation includes the effects of chirality, the off set in atomic register and the angle between the axes of the nanotubes on the thermal conductivity.

1Supported by ODOD, Third frontier RCP.

8:48AM H36.00005 Imaging single carbon nanotubes with thermal radiation, YUWEI FAN, SCOTT SINGER, RAYMOND BERGSTROM, B.C. REGAN, UCLA Department of Physics and Astronomy — We have constructed tiny light bulbs, visible to the naked eye, using individual carbon nanotubes as filaments. A nanotube is suspended over a hole in a solid silicon substrate, and is heated to incandescence with electrical current. Diffraction-limited optical microscopy identifies the nanotube position and orientation, and allows direct comparison with high-resolution transmission electron micrographs of the same nanotube. Our current progress toward quantitative pyrometry will be described.

1Currently with the UCLA Nanoelectronics Research Facility, Department of Electrical Engineering
9:00AM H36.00006 Thermal conductance and bolometric response of individual single-walled carbon nanotubes1, DANIEL SANTAVICCA, JOEL CHUDOW, ANTHONY ANNUNZIATA, LUIGI FRUNZIO, DANIEL PROBER, Dept. of Applied Physics, Yale University, MENINDER PUREWAL, PHILIP KIM, Deps. of Physics and Applied Physics, Columbia University — We describe low temperature electrothermal characterizations of individual single-walled carbon nanotubes on insulating substrates. The increase in differential resistance with increasing dc bias current is attributed to Joule heating. This is confirmed by Johnson noise thermometry, and thus the resistance can be used as a direct probe of the average electron temperature. These measurements enable us to determine the nanotube thermal conductance. We also measure the rf heterodyne response and find that the data agree well with a linear response bolometric model using our experimental value for the thermal conductance. This is the first demonstration of bolometric detection in an individual nanotube.

1This work is supported by NSF-CHE-0616875 (Yale) and NSF-DMR-0349232 (Columbia).

9:12AM H36.00007 Investigation of Optical Absorption and Thermal Transport in Suspended Carbon Nanotube Bundles . , I-KAI HSU, Department of Materials Science and Electrical Engineering, University of Southern California, ADAM BUSHMAKER, MEHMET AKYOL, STEPHEN CRONIN, Department of Materials Science and Electrical Engineering, University of Southern California, MICHAEL PETTES, LI SHI, Department of Mechanical Engineering and Center for Nano and Molecular Science and Technology, Texas Materials Institute,University of Texas of Austin — The optical absorption in suspended carbon nanotube (CNT) bundles is measured using Raman spectroscopy and two platinum resistance thermometers (PRTs), located at both ends of the suspended CNTs. The power absorbed from an incident focused laser is determined from the thermal power flowing through both ends of the CNT, detected by resistance changes in the PRTs. The results show 0.03 to 0.44% absorption of a focused 532nm laser with a 0.4µm diameter spot size incident on CNT bundles with diameters and lengths varying from 7.1-8.2nm and 11.7-14.3µm, respectively. The thermal conductance of the suspended CNT bundles can also be obtained by measuring the temperature difference between the incident laser spot and both ends of the suspended CNT. Here, temperatures in the center of the nanotube are extracted from the temperature-induced downshifts of the G band Raman mode.

9:24AM H36.00008 Terahertz Bolometric Detection in an Individual Single-Walled Carbon Nanotube1, JOEL CHUDOW, DANIEL SANTAVICCA, ANTHONY ANNUNZIATA, LUIGI FRUNZIO, DANIEL PROBER, Dept. of Applied Physics, Yale University, CHARLES SCHUMITTEMAER, Dept. of Chemistry, Yale University, PHILIP KIM, Deps. of Physics and Applied Physics, Columbia University — We describe measurements of terahertz detection in individual single-walled carbon nanotubes. The terahertz power dissipated in the antenna-coupled nanotube is determined from the induced temperature change via the nanotube’s temperature-dependent resistance. This is the first demonstration of terahertz bolometric detection in an individual nanotube. This experimental technique is being developed to study high-frequency charge excitations in the nanotube, which are predicted to display Luttinger-liquid behavior due to the lack of screening in one dimension.

1This work is supported by NSF-CHE-0616875 (Yale) and NSF-DMR-0349232 (Columbia).

9:36AM H36.00009 Quantum-dot thermometry applied to the study of electron-phonon interaction in nanowires . , JASON MATTHEWS, University of Oregon, Eugene, Oregon, HENRIK NILSSON, LARS SAMUELSON, Lund University, Sweden, HEINER LINKE, University of Oregon, Eugene, Oregon — The thermal properties of mesoscopic devices are greatly influenced by quantum and finite-size effects. For example, the influence of electron-phonon coupling on heat flow through nanowires is different than in bulk materials and has not been studied in detail. One challenging aspect of performing thermal experiments with a mesoscopic device is the application and quantification of a temperature difference across a sub-micron distance. The recently introduced quantum-dot thermometry1,2 uses a quantum dot to measure the electronic temperature difference across the dot’s dimension. We present here experimental results demonstrating quantum-dot thermometry using a quantum dot embedded in an InAs nanowire. In addition, we show result which suggest that quantum-dot thermometry can be used to measure the strength of electron-phonon interaction in a one-dimensional nanowire. 1. Hoffmann, E.A. et al., Quantum-dot thermometry, Appl. Phys. Lett. 91(25), 252114 (2007). 2. Hoffmann, E.A. et al., Measuring temperature gradients over nanometer length scales, Submitted to Nano Letters (2008).

9:48AM H36.00010 Numerical study of heat flow and electron-phonon coupling in nanowires . , JASON MATTHEWS, ERIC HOFFMANN, JASON MATTHEWS, University of Oregon, Eugene, OR, HENRIK NILSSON, LARS SAMUELSON, Lund University, Sweden, HEINER LINKE, University of Oregon, Eugene, OR — The strength of electron-phonon (e-ph) interaction in one-dimensional systems is an important mechanism that controls heat flow generated by Joule heating, e.g. in nanowires. Here we use finite element modeling to study the effects of e-ph interactions on the electron temperature profile within a heterostructure nanowire. In recent experiments, we have measured the electron temperatures in the vicinity of a double-barrier quantum dot embedded in a nanowire. We find a significant electron temperature rise in the non-heated (drain) end of the nanowire near the dot. Such a temperature rise is unexpected due to electrons seeing the dot as both electrically and thermally insulating. It is suspected that this temperature rise is due to heat bypassing the quantum dot via phonons, which in turn heat electrons in the nanowire drain by means of e-ph interaction. Our modeling results are in agreement with measured electronic temperatures, suggesting that these measurements could be used to determine the strength of e-ph interaction.

10:00AM H36.0011 Nonlinear Optical Properties of Carbon Nanotubes from First Principles . , JACK DESLIPPE, University of California at Berkeley and Lawrence Berkeley National Lab, DAVID PRENDERGAST, Lawrence Berkeley National Lab, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The optical excitation spectra of both semiconducting and metallic single-walled carbon nanotubes (SWNTs) as well as other 1D materials are dominated by exciton states of large binding energy and well defined symmetries in the group of the k-vector along the periodic direction. The optical oscillator strength is transferred almost entirely from the continuum into the excitons and the corresponding exciton-phonon states. Recent experiments have probed the spectral structure of the excited states of various symmetry in SWNTs using nonlinear optics techniques such as ultrafast spectroscopy, multi-photon spectroscopy, and phonon-assisted spectroscopy. We have developed and applied a new method based on the first-principles GW-Bethe Salpeter approach to the study of the nonlinear optical properties of the SWNTs. Supported by NSF Grant No. DMR07-05941, US DOE Contract No. DE- AC02-05CH11231 and DOE CSGF grant DE-FG02-97ER25308 and computational resources from Teragrid and NERSC.

10:12AM H36.00112 The BO Approximation Breakdown - Raman Spectroscopy of Suspended Single-Walled Carbon Nanotubes under Gate Voltages . , ADAM W. BUSHMAKER, University of Southern California, VIKRAM V. DESHPANDE, SCOTT HSIEH, MARC W. BOCKRATH, Caltech, STEPHEN B. CRONIN, University of Southern California — Since the creation of quantum dots, the BO approximation has been a useful heuristic for understanding quantum and finite-size effects. For example, the influence of electron-phonon coupling on heat flow through nanowires is different than in bulk materials and has not been studied in detail. One challenging aspect of performing thermal experiments with a mesoscopic device is the application and quantification of a temperature difference across a sub-micron distance. The recently introduced quantum-dot thermometry1,2 uses a quantum dot to measure the electronic temperature difference across the dot’s dimension. We present here experimental results demonstrating quantum-dot thermometry using a quantum dot embedded in an InAs nanowire. In addition, we show result which suggest that quantum-dot thermometry can be used to measure the strength of electron-phonon interaction in a one-dimensional nanowire. 1. Hoffmann, E.A. et al., Quantum-dot thermometry, Appl. Phys. Lett. 91(25), 252114 (2007). 2. Hoffmann, E.A. et al., Measuring temperature gradients over nanometer length scales, Submitted to Nano Letters (2008).

1This work is supported by NSF-CHE-0616875 (Yale) and NSF-DMR-0349232 (Columbia).
10:24AM H36.00013 Raman Scattering Study of Carbon Nanotube Serpentines. BEI WANG, AWNISH GUPTA, Department of Physics, Penn State University, PETER EKlund, Department of Physics, Department of Materials Science & Engineering and Materials Research Institute, Penn State University, JUN HUANG, WONBONG CHOI, Department of Mechanical and Materials Engineering, Florida International University, PENN STATE UNIVERSITY COLLABORATION, FLORIDA INTERNATIONAL UNIVERSITY COLLABORATION — Single-walled carbon nanotubes (SWNTs) were grown on step-edge single crystal quartz using CVD. SEM images were taken using FESEM showing serpentines and loops. Raman spectra were taken on SWNTs using excitation lines 514nm and 647nm with laser spot diameter ∼0.8μm. By tracing the Raman spectrum along a SWNT, we were able to record the change of Raman features with respect to the bending radius R of tube in the plane of the substrate. We found that there is linear upshift of the G-band and R-band with the curvature (1/R) of the bend. We attribute the shift of these frequencies to strain related change of carbon-carbon bond length. In semiconducting SWNTs changes were also observed in the intensities of these bands which we identify with a curvature induced change in the band-gap. This interpretation is also consistent with the results of electronic measurements.

This work is supported by NSF NIRT ECS 06-09243.

10:36AM H36.00014 Raman Spectroscopy of isolated double wall carbon nanotubes with different metallic and semiconducting configurations. FEDERICO VILLALPANDO, Department of Materials Science and Engineering, MIT, DANIEL NEZICH, Department of Physics, MIT, YOONG AHM KIM, Faculty of Engineering, Shinshu University, DAISUKI SHIMAMOTO, Faculty of Engineering, Shinshu University, HIROYUKI MURAMATSU, Institute of Carbon Science and Technology, Shinshu University, TAKUYA HAYASHI, Faculty of Engineering, Shinshu University, JING KONG, Department of Electrical Engineering and Computer Science, MIT, ENDO MORIBU, Faculty of Engineering, Shinshu University, MAURICIO TERRONES, Advanced Materials Department, IPICYT, MILDRED DRESSELHAUS, Department of Physics and 2. Department of Electrical Engineering and Computer Science, MIT — We have developed an experimental technique to obtain the Raman spectra from individual double wall carbon nanotubes (DWNt). A chemical vapor deposition (CVD) derived sample of DWNts is dispersed into solution and placed on a Si substrate. The Si substrate contains lithographic markers that allow us to record the exact location of individual and isolated DWNts and obtain their Raman spectra with various laser energies. The laser energy can be in resonance with the inner and/or the outer layers of the same DWNT. We report on the differences between individual DWNTs with different metallic and semiconducting configurations and compare our results to previous experiments performed on DWNT bundles.

CONACYT Mexico and NSF DMR-0704197.

10:48AM H36.00015 Softening of the Radial Breathing Mode in Metallic Carbon Nanotubes. HOOTAN FARHAT, MIT, KEN-ICHI SASAKI, Hiroshima University, MARTIN KALBAC, Academy of Sciences of the Czech Republic, MARIO HOFMANN, MIT, RIICHIRO SAITO, Tohoku University, MILDRED S. DRESSELHAUS, JING KONG, MIT — In this work, the Fermi level (εF) dependence of the radial breathing mode (RBM) of metallic single walled carbon nanotubes (M-SWNTs) has been investigated. In situ Raman spectra were obtained from several individual M-SWNTs while varying εF electrochemically. The RBM frequency of an intrinsic M-SWNT is shown to be downshifted relative to highly doped tubes by ∼2 cm⁻¹. The downshift is greatest for small diameter and small chiral angle nanotubes. Most tubes do not show any change in RBM linewidth. A comparison is drawn between the RBM and the G-band (A₁LO phonon) with respect to the εF dependence of their frequencies and linewidths.

Tuesday, March 17, 2009 8:00AM - 11:00AM — Session H37 DCP: Focus Session: Spectroscopic Probes of Biomolecular Structure and Function I 409

8:00AM H37.00001 Structure and dynamics in B12 enzyme catalysis revealed by electron paramagnetic resonance spectroscopy. KURT WARNCKE, Emory University — Challenges to the understanding of how protein structure and dynamics contribute to catalysis, and the use of time-resolved electron paramagnetic resonance (EPR) spectroscopic techniques to address the challenges, are examined in the context of the cobzyme B12-dependent enzyme, ethanalamine ammonia-lyase (EAL), from Salmonella typhimurium. EAL conducts the homolytic cleavage of the coenzyme cobalt-carbon bond, intraprotein radical migration (5-6 Å), and hydrogen atom transfers, which enable the core radical-mediated rearrangement reaction. Thermodynamic and activation parameters are measured in two experimental systems, which were developed to isolate sub-sequences from the multi-step catalytic cycle, as follows: (1) A dimethylsulfoxide (DMSO)/water cryosolvent system is used to prepare the kinetically-arrested enzyme/coenzyme/substrate ternary complex in fluid solution at 230 K.[1] Temperature-step initiated cobalt-carbon bond cleavage and radical pair separation to form the Co(II)-substrate radical pair are monitored by using time-resolved, full-spectrum EPR spectroscopy (234°C<T≤250 K).[1] (2) The Co(II)-substrate radical pair is cryotrapped in frozen aqueous solution at T<150 K, and then promoted to react by a temperature step. The reaction of the substrate radical along the native pathway to form the diamagnetic bound products is monitored by using time-resolved, full-spectrum EPR spectroscopy (187°C<T≤217 K).[2] High temporal resolution is achieved, because the reactions are dramatically slowed at the low temperatures, relative to the initiation and spectrum acquisition times. The results are combined with high resolution structures of the reactant centers, obtained by pulsed-EPR spectroscopies.[3] and the protein, obtained by structural proteomics[4] and EPR and electron spin echo envelope modulation (ESEEM) in combination with site directed mutagenesis,[5] to approach a molecular level description of protein contributions to catalysis in EAL.


1Supported by NIH grant DK54514.
8:36AM H37.00002 Time-resolved X-ray scattering of proteins in solution: a new method for probing biomolecular structure and function
We thank Bill Royer, John Olson, and Jayashree Soman for providing protein samples used in these studies. This research was supported in part by the Intramural Research Program of the NIH, NIDDK.

9:12AM H37.00003 Ultrafast Photodynamics in Diverse DNA Structures from A-tracts to Z-DNA
BERNH KOHLER, Department of Chemistry, The Ohio State University — The vulnerability of the genome to UV photodamage has sustained interest in excited electronic states in DNA for over 50 years. Progress in understanding the nature and dynamics of electronic excitations in DNA has accelerated rapidly thanks in part to ultrafast spectroscopy. Most excitations in single DNA bases decay nonradiatively in hundreds of femtoseconds. Surprisingly, much longer-lived excited states are observed in femtosecond pump-probe experiments on single- and double-stranded DNAs. Localized charge transfer states are prominent in runs of adenine bases (A tracts). DNA is polymorphic and can adopt a range of structures beyond the iconic B-form double helix. The effect of helix conformation on excited-state dynamics has been studied in a double-stranded oligonucleotide that can be switched between B- and Z-forms. Experiments on G quadruplex structures and on i-motif DNA reveal that these forms have significantly slower relaxation than B-DNA. By altering π − π stacking and hydrogen bonding, structure profoundly affects the complex photoprocesses observed in DNA.

3 This work was supported by grants from NSF and NIH.

9:48AM H37.00004 Charge Transfer States of Aqueous B-DNA at Energies Above the Bright Exciton States
ADRIAN LANGE, Chemistry Dept. (Physical), JOHN HERBERT, Chemistry Dept. — Charge transfer states have been proposed to explain experimentally observed long-lived excited states in aqueous DNA oligomer[1]. Due to the large number of atoms, tractably describing such excited states in DNA systems with ab initio theory is limited to TD-DFT. However, standard TD-DFT exchange-correlation functionals significantly underestimate CT excitation energies owing to incorrect asymptotic behavior. To circumvent this error, we instead apply recently developed and optimized long-range corrected TD-DFT functionals to better assess the low lying CT and exciton states of DNA oligomers. We show that long-range corrected TD-DFT yields results comparable to correlated wave function models, placing CT states of aqueous B-DNA at energies above the optically bright 1ππ* exciton states, contrary to TD-DFT results which find CT states below the exciton states.


10:00AM H37.00005 Low frequency dynamics of Cytochrome c
KARUNAKARAN VENUGOPAL, PAUL CHAMPION, Department of Physics and Center for Interdisciplinary Research on Complex System, Northeastern University, Boston — Femtosecond coherence spectroscopy is used to investigate the low frequency dynamics of cytochrome c (cyt c). There is good agreement between the higher frequency oscillatory components of the coherence spectra and the low frequency Raman spectra. A mode near ~40 cm⁻¹ is a universal feature of heme systems and has been assigned to doming motions that are strongly enhanced upon ligand photolysis [1]. A dominant heme ruffling mode near ~60 cm⁻¹ [2] appears in ferric cyt c for excitation in the region 425-432 nm, to the red of the Soret maximum (408 nm). This, along with a phase jump of ~ π in this region, suggests the ruffling mode is coupled to a charge transfer (CT) band underlying the Soret band [3] and that it is a potentially important electron transfer reaction coordinate. [1] F. Gruia, M. Kubo, X. Ye, P. M. Champion, Biophys. J., 2008, 94, 2252. [2] M. Kubo, F. Gruia, A. Benabas, A. Barabanschkov, W. R. Montfort, E. M. Maes, P. M. Champion, J. Am. Chem. Soc., 2008, 130, 9800. [3] K. T. Schomacker, P. M. Champion, J. Chem. Phys., 1986, 84, 5314.

10:12AM H37.00006 Ultrafast Dynamics of Leu-Enkephalin in Water and Membranes
SOOHWAN SUL, YUAN FENG, UYEN LE, NIEN-HUI GE, Department of Chemistry, University of California, Irvine — Ultrafast two-dimensional infrared (2D IR) spectroscopy has been applied to investigate the peptide-membrane interaction and conformational distribution of Leu-enkephalin (Lenk) in bilayer membranes. We compare the results from linear and 2D IR experiments on p-cresol in water, Lenk in water, and Lenk in membranes, focusing on the ring stretching mode of the Tyr side chain. Frequency-frequency correlation functions obtained from a series of waiting-time-dependent 2D IR spectra reveal a fast decaying component with a ~1 ps time constant that is common for all three systems. This spectral diffusion component is attributed to hydrogen-bond making-breaking dynamics of the Tyr side chain. Unlike p-cresol in water, both Lenk systems exhibit substantial spectral inhomogeneity that does not decay within the 4 ps window. The observed hydrogen-bond dynamics suggests that the Tyr side chain of Lenk in membranes is located at the water-abundant region at the water-membrane interface. The experimental results are compared with those from MD simulations and DFT calculations.

1 Partially supported by NSF.

10:24AM H37.00007 Flap Conformations in HIV-1 Protease are Altered by Mutations
GAIL FANUCCI, MANDY BLACKBURN, ANGELO VELORO, LUIS GALIANO, University of Florida, DING FANGU, CARLOS SIMMERLING, Stony Brook — HIV-1 protease (PR) is an enzyme that is a major drug target in the treatment of AIDS. Although the structure and function of HIV-1 PR have been studied for over 20 years, questions remain regarding the conformations and dynamics of the β-hairpin turns (flaps) that cover the active site cavity. Distance measurements with pulsed EPR spectroscopy of spin labeled constructs of HIV-1 PR have been used to characterize the flap conformations in the apo and inhibitor bound states. From the most probably distances and the breadth of the distance distribution profiles from analysis of the EPR data, insights regarding the flap conformations and flexibility are gained. The EPR results clearly show how drug pressure selected mutations alter the average conformation of the flaps and the degree of opening of the flaps. Molecular dynamics simulations successfully regenerate the experimentally determined distance distribution profiles, and more importantly, provide structural models for full interpretation of the EPR results. By combining experiment and theory to understand the role that altered flap flexibility/conformations play in the mechanism of drug resistance, key insights are gained toward the rational development of new inhibitors of this important enzyme.
10:36AM H37.00008 An Investigation of Ionic Binding to Fatty Acid Monolayers by Broad-bandwidth Sum Frequency Generation Vibrational Spectroscopy1, CHENG TANG, HEATHER ALLEN, Ohio State University — Model study of ionic binding of fatty acid monolayer is a good proxy towards understanding the fundamental chemistry in biological processes. In this study, we used broad-bandwidth sum frequency generation (BBSFG) vibrational spectroscopy to investigate the ionic binding event that leads to deprotonation of the fatty acid head groups. Palmitic acid (C15C00H) exists as monolayer on aqueous surfaces, and on aqueous alkali and alkaline solutions surfaces. Surface vibrational stretching modes of palmitic acid from 1400 cm$^{-1}$ to 3700 cm$^{-1}$ were observed (COO$^*$, C=O, C-H, and O-H). Palmitic acid is mostly protonated at the aqueous surface at neutral pH ($\sim$6). However, various degrees of deprotonation are initiated by introduction of different cations in the salt solutions albeit at neutral pH.

1 NSF Chemistry Grant (analytical and surface science div.)

10:48AM H37.00009 Using Rotationally Resolved Electronic Spectroscopy to Probe Chiral Molecules in the Gas Phase1, JUSTIN YOUNG, LEONARDO ALVAREZ-VALTIERRA, DAVID PRATT, University of Pittsburgh — It is well established that biological processes involving chiral molecules can show a preference of one enantiomer relative to the other. Reported here are high resolution spectroscopy experiments that allow one to distinguish one diastereomer from another, and thereby establish if the structural requirements for diastereoisomeric present.

1 Work supported by NSF (CHE-0615755)

Tuesday, March 17, 2009 8:00AM - 10:48AM –
Session H38 DCP: Focus Session: Theory of Electron Transport Through Molecules I

8:00AM H38.00001 The Role of Symmetry in Molecular Electronic Conduction, JEFFREY REIMERS, University of Sydney, Australia — The Greens Function Density-Functional Tight-Binding (gDFTB) method is applied to determine the role that molecular symmetry plays in single-molecule conductivity. Both coherent elastic electron transport and inelastic electron-tunnelling spectroscopy (IETS) are considered. Symmetry becomes manifest in various ways: through the molecular point-group symmetry of the conducting molecule (D2h, for chemisorbed benzenedithiol between two gold electrodes), through the conductance point-group symmetry displayed by the gDFTB equations (this embodies junction symmetry and may be very low and nominally non-existent), and through an approximate molecular-conductance point group (C2h, for chemisorbed benzenedithiol). Indeed, the conductivities for a range of relevant problems are well approximated using the restriction of molecular-conductance point-group. This allows the complex transmission curves calculated by many research groups to be dramatically simplified and partitioned into symmetry-depicted channels. Means are introduced that isolate a very small number of component channels describing different aspects of single-molecule conductivity: input junction channels, through-molecule channels, and output-junction channels. For elastic transport, all through-molecule channels are totally symmetric and hence a rigorous selection rule appears that transport is allowed involving only input-junction and output-junction channels of the same symmetry. However, for IETS, the through-molecule channels have the symmetry of the scattering molecular vibration and hence the input-junction and output-junction channel symmetries may vary. In general, just one channel is expected to dominate the junctions, leading to the IETS propensity rule that totally symmetric transitions are the most intense ones. Simple physical pictures are presented showing the input, vibrational scattering, and output channels for IETS, leading to predictions of how this effect can be controlled chemically.

8:36AM H38.00002 Molecular and Nano Scale Device-conductance: steady state and dynamical analysis, BARRY D. DUNIETZ, University of Michigan — A computational approach is used and developed to study electron transport through molecular and nano scale devices. New models and methods are employed to describe the dynamics of electron transport under the influence of time dependent (TD) perturbations. Quantum interferences affecting the TD conductance are analyzed for transient aspects, effects of present bound states and transport under the effect of coherent excitations. I will also discuss our modeling of several recent high-profile experimental studies achieving molecular scale (steady state) conductance which provides intriguing insight at the molecular structural level on the functionality of the conducting devices. The studies involve metal recognition properties of short peptides or fabricated molecular sockets based on surface confined terpyridine ligands. If time permits I will describe the required structural features for a gating field to tune the conductance of a molecular conjugated system.

9:12AM H38.00003 The spectroscopic dynamics of electron transport through molecular junctions, ALEXANDER PROCIUK, BARRY DUNIETZ, University of Michigan — A non-equilibrium Green’s-Function (NEGF) model based on time dependent perturbation theory is developed to compute the spectroscopic dynamics of electron transport through molecular junctions under the influence of weak time dependent classical fields. In this model, we use the two time variable nature of the Kadanoff-Baym equations of motion to formulate a mixed time-frequency representation for the electronic density. The resulting highly informative time dependent Wigner distributions are used to shed light on the features of dynamical observables, such as electron current, dipole moment and population. We analyze laser induced coherence and population transfer effects for both Markovian and non-Markovian electrode models. If time permits, the analysis of transient conductance with respect to the system’s fundamental parameters will be discussed.

9:24AM H38.00004 Model ab initio studies of solvation and excess charge localization on conjugated carbon chains1, MICHAEL MAYO, YURI GARTSTEIN, The University of Texas at Dallas — Using long C$_n$H$_{2n}$ conjugated carbon chains with the polymeric structure as prototypical examples of one-dimensional (1D) semiconductors, we discuss self-localization of excess charge carriers in the presence of the interaction with a surrounding polar solvent. The solvation mechanism of self-trapping is different from the self-localization due to coupling with bond-length modulations of the underlying atomic lattice well-known in conjugated polymers. Model ab initio computations are carried out and compared that employ various methods such as hybrid density functionals and Hartree-Fock within the framework of the polarizable continuum model. We demonstrate the possibility of the formation of large 1D electron- and hole-polarons entirely due to solvation, but even larger degrees of charge localization occur when accompanied by atomic displacements. Also discussed are doubly-charged bipolaron states and topological kink-solitons that may be formed in these systems. For a brief report, see M. L. Mayo and Yu. N. Gartstein, Phys. Rev. B 78, 073402 (2008).

1 We are grateful to the Collaborative U. T. Dallas-SPRING Research and Nanotechnology Transfer Program for financial support
9:36AM H38.00005 Measuring single electron charging energy in self-assembled single nanoparticle devices: Coulomb blockade threshold vs. Arrhenius energy, AL-AMIN DHIRANI, AMIR ZABET-KHOSOUSI — Single-nanoparticle (NP) devices formed by self-assembling NPs onto alkanedithiol-functionalized break junctions exhibit Coulomb blockade (CB) conductance suppressions at low temperatures. We have studied temperature dependence of conductance inside the CB region and find multiple activation energies ($E_a$): A small $E_a$ at low temperatures, and a larger $E_a$ at high temperatures. The small $E_a$ is independent of NP size and is attributed to an energy state located at the metal–molecule contact. The larger $E_a$ scales with NP size and is attributed to single electron charging energy of the NPs. Importantly, we observe a significant (~5–100 fold) discrepancy between values of charging energies obtained from CB voltage thresholds and $E_a$. To account for the discrepancy, we propose a model in which electrons are temporarily localized at the energy states near the metal–molecule interface and lose energy. The proposed model is supported by ultraviolet photoelectron spectroscopy of alkanedithiol monolayers on gold which indicates a presence of energy states close to the Fermi level of gold likely arising from gold–thiolate bonds. A suitably modified Orthodox theory successfully describes our measurements.

9:48AM H38.00006 Molecular transport in the language of many-body states, MICHAEL GALPERIN, UCSD — Recent advancements in experimental techniques at nanoscale caused a surge in research of transport through molecular junctions. Nonlinearity of current-voltage characteristic at resonance makes this regime particularly important for potential molecular based memory, switches and logic devices. One of important differences of molecular junctions (compared e.g. to semiconductor QDs) is sensitivity of electronic and vibrational structure of the molecule to oxidation/reduction of the molecule. This implies necessity of treating the transport at resonance in the language of molecular states rather than single particle orbitals. The latter are the choice of majority of available ab initio approaches. We consider two possible schemes capable of incorporating isolated molecule (many-body) states as a basis for transport calculations. The schemes utilize Hubbard operators for description of single electron transitions between many-body states and go beyond previously proposed scattering theory and standard quantum master equation approaches.

10:00AM H38.00007 WKB modeling of single molecular transport and Molecular Nanometrology, VLADIMIR BURTMAN, Physics and Geophysics Department, University of Utah, SLC, ANDREI V. PAKOULEV, Department of Chemistry, University of Wisconsin, Madison — Wentzel–Kramers–Brillouin (WKB) approach to model transport mechanism in molecular nanostructures is discussed in context of molecular nanometrology. Two WKB models, direct tunneling (Simmons model) and field emission tunneling (Fowler-Nordheim tunneling), could be used to model conductivity in single molecular structure at low and elevated biased. Potentially, Simmons model could extract two molecular barriers, one for electrons and one for holes from conductivity spectra. Following this assumption electrical and optical gap-probed molecular nanometrology (GMN) could be developed. The main GMN principle is the small difference between the values of the HOMO-LUMO energy gap detected by electrical and optical measurements. We will compare experimentally derived electrical and optical probed gap and energy offsets between $E_F$ and nearest molecular orbital to discuss applicability and feasibility of this approach. 

1. A. Pakoulev acknowledges support from NSF grant CHE0650431.


10:24AM H38.00009 Theoretical study of electron transport through $\pi$-stacked ethylbenzene lines bonded to a Si surface, MANUEL SMEU, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, QC, Canada, ROBERT WOLKOW, National Institute for Nanotechnology and Department of Physics, University of Alberta, Edmonton, AB, Canada, HONG GUO, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, QC, Canada — Recently, experimental techniques were developed for lines of $\pi$-stacked ethylbenzene molecules to self-assemble on an H-terminated Si (100) surface in the laboratory of one of the authors. In this work, we use density functional theory (DFT) combined with the nonequilibrium Green’s function formalism (NEGF) to model electron transport through these ethylbenzene lines to determine if they could be used as molecular wires. In our calculations, the molecules are bonded to an H-terminated Si (100) surface and are bridging two Al leads. The transmission spectrum and its associated scattering states are determined by the NEGF-DFT technique. The presence of the Si substrate is found to play an important role for conduction: there is a dominant transmission peak near the Fermi level which is contributed by the Si substrate and not the $\pi$-stacked molecular line. The low-bias resistance is found to increase exponentially with the length of the molecular line, indicating a tunneling behavior in conduction.

10:36AM H38.00010 Stark Spectroscopy of Conjugated Oligomers and Polymers Important for Organic Devices, ALBERTO MOSCATELLI, DAVID C. COPPOCK, LINDA A. PETEANU, Carnegie Mellon University — Fluorescent conjugated oligomers, have been tested using this approach. Comparison of the results from single chains and from aggregates reveal how intermolecular interactions impact charge transfer and electronic delocalization in these technologically-important systems.
8:00AM H39.00001 A New Mechanism for Domain Size Selection in Curved Lipid Membranes\(^1\),
FANGFU YE, JONATHAN SELINGER, Kent State University — Lipid membranes, composed of saturated lipids, unsaturated phospholipids and cholesterol, play important roles in maintaining cellular activities. It is now well established that lipid membranes under proper conditions separate into saturated-lipid-enriched (L\(_o\)) phase regions and unsaturated-lipid-enriched liquid-disordered (L\(_d\)) phase regions, with the L\(_o\) phase having a larger bending modulus than the L\(_d\) phase. In this project, we study how the bending modulus difference between L\(_o\) and L\(_d\) phases may affect the phase separation behavior of uniformly curved lipid membranes. We believe that, for a spherical lipid vesicle, when the line tension and phase transitions are in the gel state, (i.e.: their acyl chains have a ~32 degree azimuthal tilt with respect to the membranes normal), the membrane as a uniaxial crystal would be able to change the position of the acyl chains by measuring the birefringence and optical orientation. By controlling the temperature of our sample we hope to better study the curvature changes that occur during phase transitions from gel to liquid states. The investigation of other lipid mixtures and the transformations they undergo during different phases will also be discussed.

\(^1\)Supported by ICAM and NSF Grant DMR-0605889

8:12AM H39.00002 Making Sense of the Polymorphous Shapes of Giant Liposomes, YAN YU, Dept of Materials Science and Engineering, Univ of Illinois-Urbana Champaign, STEPHEN ANTHONY, Dept of Chemistry, Univ of Illinois-Urbana Champaign, JULIE VROMAN, SUNG CHUL BAE, Dept of Materials Science and Engineering, Univ of Illinois-Urbana Champaign, STEVE GRANICK, Dept of Materials Science and Engineering, Physics, Chemistry and Chemical Engineering, Univ of Illinois-Urbana Champaign — Lipid vesicles, especially giant unilamellar vesicles (GUVs) are often used as simplified models for biological membranes, but their polymorphous panoply of shapes and shape changes is notorious to those who work with them. This affords opportunities to study why phospholipid membranes so often fail to minimize their surface area to adopt spherical shapes. Instabilities can be triggered by the tension caused by optical tweezers, osmotic perturbations, or polymer anchorage. This talk will describe the evolution of GUVs from spherical to pearl-like and to tube-like shapes, and back again reversibly.

8:24AM H39.00003 Near-Field structural studies of lipid bilayers, MERRELL JOHNSON, RICARDO DECCA, IUPUI Physics Dept. — We use a Near-field Scanning Optical Microscope (NSOM) in conjunction with a Photo Elastic Modulator (PEM) to conduct birefringence measurements with a spatial resolution of ~80nm. With our current setup we are able to distinguish changes in retardance \(\alpha = \frac{2\pi(n_0-n_e)}{\lambda}\) on the order of \(5 \times 10^{-3}\) radians. Simultaneously while gathering information about \(\alpha\) we extract information about the samples optical orientation \(\theta\), reference to the sample’s axis, with an accuracy of \(3.64 \times 10^{-3}\) radians. We use our system on 1,2-dipalmitoylphosphatidylcholine (DPPC) bilayers, which at room temperature are in the gel state. (i.e.: their acyl chains have a ~32 degree azimuthal tilt with respect to the membranes normal). Modeling the membrane as a uniaxial crystal we are able to determine the position of the acyl chains by measuring the birefringence and optical orientation. By controlling the temperature of our sample we hope to better study the curvature changes that occur during phase transitions from gel to liquid states. The investigation of other lipid mixtures and the transformations they undergo during different phases will also be discussed.

8:36AM H39.00004 X-ray insight into cholesterol-phospholipid interactions, DAVID GIDALEVITZ, Division of Physics, BCPS department, CMoS, Illinois Institute of Technology, Chicago, IL, USA — The mechanism of nonideal cholesterol-lipids mixing yet remains controversial. We report on a systematic study of cholesterol-phospholipid interactions in lipid monolayers using Langmuir isotherms, synchrotron X-ray reflectivity (XR), and grazing-incidence X-ray diffraction (GIXD) techniques. Lipid monolayers consisted of cholesterol-DPPC mixtures with cholesterol mole fractions \(\chi_{CHOL}\), varying from 0 to 1. GIXD reveals that at both \(\chi_{CHOL}\) and \(\chi_{DPPC}\) above 85 mixed films exhibit packing order of a prevalent lipid. In between, cholesterol seizes places in DPPC crystalline lattice at the stoichiometry. Similar to that of the mixture inducing short-range regular-hexagonal packing order with increasing spacing between molecules as a function of cholesterol content. XR shows that cholesterol tends to stay in DPPC acyl chains at low \(\chi_{CHOL}\) while gradually descending to a subphase at higher \(\chi_{CHOL}\) accompanied by rearrangement of DPPC headgroups. Thus, a desire of highly nonpolar cholesterol to avoid contacts with polar water molecules and/or DPPC headgroups defines a mode of cholesterol-lipid interactions.

8:48AM H39.00005 ABSTRACT WITHDRAWN

9:00AM H39.00006 Monte Carlo Simulation of Coexisting Phases in DOPC/DSPC/Cholesterol Ternary Mixtures, REJWAN ALI, Polytechnic Institute of New York University, JIAN DAI, JUYANG HUANG, Texas Tech University — Lipid raft domain will open up path for modeling many cellular phenomena. Extensive studies on model raft consists of DOPC/DSPC/cholesterol ternary system have been reported by many experimental groups. We report Monte Carlo simulation to reconstruct experimental phase diagram. Both pair-wise and multi-body interactions have been used to simulate the phase boundary of liquid-ordered phase and liquid-disordered phase coexistence region. A new algorithm, named the "Composition Evaluation Method," was implemented to determine the compositions of the coexisting phases in simulations. The new method is about 20~50 times faster in determining phase boundaries, comparing to the traditional free energy calculation. In addition, pair correlation functions were used to map the phase boundaries in the critical region. We found that pair-wise interactions can reproduce the experimental critical point as well as the slope of tie lines, but not the compositions of the coexisting phases. Simulations with multi-body interactions produced a much better fit to the experimental phase diagram.

9:12AM H39.00007 Structural studies of mixed lipid bilayers on solid substrates using x-ray reflectivity, GANG CHEN, MINMAY MUKHOPADHYAY, YICONG MA, SUNIL SINHA, Department of Physics, University of California, San Diego, ZHANG JIANG, Advanced Photon Source, Argonne National Laboratory, CURT DECARO, JUSTIN BERRY, LAURENCE LURIO, Department of Physics, Northern Illinois University, ADRIAN BROZELL, ATUL PARIKH, Departments of Applied Science and Biophysics Graduate Group, University of California, Davis — The lipid bilayers of natural membranes generally exist in a fluid state which occurs above the gel to liquid crystalline phase transition temperature. Knowledge of the structure of such bilayers is important for understanding fundamental biological processes mediated by or occurring within membranes. We have performed systematic measurements on bilayers of 1,2-Dipalmitoyl-sn-Glycero-3-Phosphoethanolamine (DPPE) and its mixture with 1,2-Dioleoyl-sn-Glycero-3-Phosphocholine (DOPC) and cholesterol (CH) on silicon substrates with x-ray reflectivity both below and above their phase transition temperatures. Structural variations as a function of temperature are demonstrated by fitting the reflectivity data with both a model dependent and a model independent routine. Studies of Au nanoparticle labeled DOPC and DOPC + DPPE + CH mixture are also performed and the location of Au nanoparticles in these bilayers is established by analyzing the x-ray reflectivity data.

9:24AM H39.00008 Cellular adhesion and dynamic membrane tether extraction, SARAH NOWAK, TOM CHOU, UCLA — We consider the energetics and dynamics of pulling a ligand bound to an integral membrane receptor. Deformation of the cell membrane and cytoskeleton is considered as the ligand is pulled. We assume that deformation of the cytoskeleton obeys Hook’s law up to a critical force at which the cell membrane locally detaches from the cytoskeleton and a membrane tether forms. Depending on the pulling velocity and force, a membrane tether of varying length may form before the receptor-ligand bond breaks. We study the probability of tether formation and the mean tether length at the moment of ligand detachment as a function of system parameters. This problem is applicable to AFM studies of cellular adhesion molecules, and to the biological problem of leukocyte rolling.
9:36 AM H39.00009 Lipid Micromechanics: Tethers and Fingers in membrane, LOBAT TAYEBI, UCdavis, Applied Science Department, GREGORY MILLER, ATUL PARIKH, UCdavis, Department of Applied Science — A significant body of evidence now links local mesoscopic structure (e.g., shape and composition) of the cell membrane with its function; the mechanisms by which cellular membranes adapt the specific shapes remain poorly understood. Among all the different structures adopted by cellular membranes, the tubular shape is one of the most surprising one. While their formation is typically attributed to the reorganization of membrane cytoskeleton, many exceptions exist. We report the instantaneous formation of tubular membrane mesophases allowing the hydration under specific thermal conditions. The shapes emerge in a bimodal way where we have two distinct diameter ranges for tubes, ~20µm and ~1µm, namely fat fingers and narrow tethers. We study the roughening of hydrated drops of 3 lipids in 3 different spontaneous curvatures at various temp. and ion strength to select the dominant effect in formation of tethers and fingers. Dynamics of the tubules are of particular interest where we observe four distinct steps of birth, coiling, uncoiling and retraction with different lifetime on different thermal condition. These dynamics appear to reflect interplay between membrane elasticity, surface adhesion, and thermal or hydrodynamic gradient.

9:48 AM H39.00010 Pseudo-phase Diagram of Cholesterol-Rich Filamentous, Helical Ribbon, and Crystal Microstructures, Y.A. MIROSHNIKOVA, M. ELSENBECK, GUANQING OU, Y.V. ZASTAVKER, Olin College, K. KASHURI, G.S. IANNACCHIONE, WPI — Optical and calorimetric techniques are employed to study temperature and concentration dependence of three self-assembled microstructure types formed in Chemically Defined Lipid Concentrate (CDLC): filaments, helical ribbons, and crystals. CDLC consists of cholesterol, bilayer-forming amphiphiles, and micelle-forming amphiphiles in water, and is considered to be a model system for cholesterol crystallization in gallbladder bile. Phase contrast and DIC microscopy indicate the presence of all three microstructure types in all samples studied. Optically observed structural evolution indicates that filaments first bend to form helical ribbons followed by clustering and “straightening” of these structures into short and increasingly thickening filaments that dissolve with increasing temperature. Complementary calorimetric studies (differential-scanning and modulation) reveal thermal signatures that correspond to this observed structural evolution, which occurs throughout a large region of metastable chemical coexistence. These results suggest that a pseudo-phase diagram for the microstructures formed in CDLC may be developed to explain the observed behavior of the system.

10:00 AM H39.00011 PTEN interaction with tethered bilayer lipid membranes containing PI(4,5)P2, R. MOLDOVAN, S. SHENOY, P. SHEKHAR, A. KALINOWSKI, Carnegie Mellon University, A. GERICKE, Kent State University, F. HEINRICH, M. LOESCHE, Carnegie Mellon University — Synthetic lipid membrane models are frequently used for the study of biophysical processes at cell membranes. The tethered bilayer lipid membrane (tBLM) model, based on a (C14)2(PEO)8-thiol anchor, WC14 [1]. Such membranes can be prepared to contain single phospholipids or complex lipid mixtures [2], including functional lipids involved in cell signaling, such as the highly charged phosphatidylinositol phosphates (PIPs). To study the interaction between the tumor suppressor PTEN (phosphatase and tensin homologue deleted on chromosome 10) and model membranes we have incorporated phosphatidylinositol-4,5-bisphosphate (PI(4,5)P2) in tBLMs and use fluorescence correlation spectroscopy (FCS), neutron reflectometry (NR) and surface plasmon resonance (SPR) for their characterization. NR shows that tBLMs formed with PI(4,5)P2 are complete. FCS of labeled PI(4,5)P2 shows that diffusion occurs at the time scale characteristic of membrane-incorporated lipid. Finally, SPR shows specific binding of PTEN to the model membrane thus confirming the incorporation of PI(4,5)P2 into the tBLM. [1] McGillivray et al, Biointerphases 2, 21-33 (2007) [2] Heinrich et al, Langmuir, submitted

10:12 AM H39.00012 Subdiffusion and diffusion of lipid atoms and molecules in phospholipid bilayers, ELIHU FLENNER, Colorado State University, JHUMA DAS, MAIKEL RHEINSTADTER, IOAN KOZSTIN, University of Missouri-Columbia — We examine the dynamics of lipid atoms and molecules using a 0.1 µs all-atom molecular dynamics simulation of a hydrated diyristoyl-phosphatidylcholine (DMPC) lipid bilayer. We identify three well separated time regimes in the mean square displacement, ⟨δr²(t)⟩, of the lipid atoms and molecules: (1) a ballistic regime for t < 10 femtoseconds; (2) a subdiffusive regime where ⟨δr²(t)⟩ ~ t^β and β < 1 for times between 10 picoseconds and 10 nanoseconds; and (3) a Fickian diffusion regime where ⟨δr²(t)⟩ ~ t for t > 30 nanoseconds. We propose a memory function approach for describing the mean square displacement over the whole time range, and find that the lateral self diffusion coefficient found from the memory function approach agrees well with the one determined from the mean square displacement. We use the cumulant expansion of the self-intermediate scattering function to connect the three time scales in the mean square displacement to the interpretation of neutron scattering signals.

10:24 AM H39.00013 Suppression of fluid membrane fluctuations by a periodic pinning potential: Applications to red blood cells, MARK L. HENLE, School of Engineering and Applied Sciences, Harvard University, ALEX J. LEVINE, Department of Chemistry and Biochemistry, University of California, Los Angeles — The membrane of the red blood cell (RBC) is tethered to a two-dimensional triangular network of semi-flexible elastic spectrin filaments. This network allows the cell to maintain its structural integrity during the large shape deformations that occur as it circulates through the microcirculation. The lipid membrane is anchored to the spectrin filaments at the nodes of the network. Consequently, these attachments impose a two-dimensional periodic pinning potential upon the membrane. In this talk, we investigate the effect of this pinning potential on the thermal bending fluctuations of the membrane. We show that there is an exact mapping of this system onto the classic problem of non-interacting electrons subject to a periodic potential; we exploit this mapping to obtain an exact analytic solution for a defect-free triangular array of harmonic pinning sites. The pinning potential affects both the local and global structure of the bending fluctuations. To investigate the local structure we consider the bending correlations between two nearby points in the membrane, while for the global structure we consider the total area stored in the fluctuations. We also investigate the effective area modulus of the membrane/spectrin composite structure.

10:36 AM H39.00014 Rough-Smooth-Rough Interface transition in a supported lipid bilayer system, PIYUSH VERMA, NICK MELOSH, Stanford University — Dynamic evolution of interfaces with quenched disorder is common in nature including fluid flow in porous media, granular particle flow and bacterial colony growth. These interfaces, which are either modeled using the Quenched-KPZ equation or the Quenched-Edward-Wilkinson (QEW) equation, expand due to a driving force while the edge profile roughens monotonically over time due to a distribution of disordered trapping defects. We studied interface evolution of a supported phospholipid bilayer, which is an ideal two dimensional viscoelastic material. Surprisingly, we observed a unique rough-smooth-rough bilayer interface transition on chromium oxide which has never been reported before. This transition was found to be a result of the viscoelasticity of the lipid bilayer and could be modeled using a modified QEW equation, which includes a spring-like term to account for the bilayer elasticity.

10:48 AM H39.00015 The effect of curvature on the undulation spectrum of Red Blood Cell membranes, TATIANA KURIABOVA, University of Colorado, Boulder, MARK L. HENLE, Harvard University, ALEX J. LEVINE, University of California, Los Angeles — The human red blood cell (RBC) membrane has a composite structure of a fluid lipid bilayer tethered to an elastic 2D spectrin network. The study of the mechanical properties of RBCs is crucial to our understanding of their ability withstand large amplitude deformations during their passage through the microcirculation. The linear mechanical response of this composite membrane can be measured by observing its undulatory dynamics in thermal equilibrium, i.e. micro rheology. Previous models of these dynamics postulated an effective surface tension. In this talk, we show that surface tension is not necessary. Rather, the coupling of membrane bending to spectrin network compression by curvature can account for the observed dynamics. We use a simplified theoretical model to describe the undulatory dynamics of RBCs, measured experimentally by the Popescu group. Analyzing their data using our model, we observe dramatic changes in RBC membrane elasticity associated with cells’ morphological transition from discocytes to echinocyte to spherocyte.

1G. Popescu et al. “Imaging red blood cell dynamics by quantitative phase microscopy, Blood Cells, Molecules, and Diseases, (2008), in print”
8:00AM H40.00001 Application of EPR studies on Biologically Important Copper Acetyl Acetonate and Copper Tetraphenyl Porphine via Bayesian Inference and Density Functional Theory, LAXMAN MAINALI, INDIRA SAHU, KEITH EARLE, SUNY Albany — Quantitative lineshape analysis can allow one to infer information about spin probe structure and dynamics. Experiments were performed at different frequencies (S, X, K, and W Band) for Copper acetyl acetonate (Cu(acac)$_2$) and 5,10,15,20- Tetrathenyl - 2H,23H-porphine copper(I) (CuTPP) in toluene at different temperatures. In order to obtain unbiased estimates of model parameters within the context of a given model, EPR spectra were analyzed via methods of Bayesian Inference. Four different sets of model parameters used to describe cw EPR spectra for two different probe symmetries (axial and rhombic) were explored using a model for rotational diffusion that was analyzed via Stochastic Liouville Equation. The optimized magnetic and dynamic tensor parameters were inferred from individual and simultaneous multifrequency fits and were compared with the values obtained from density functional theory (DFT). The isotropic g values estimated with PW1PW for Cu(acac)$_2$ and CuTPP with the respective basis sets 6-31G and 6-31G(d) agree well with the experimental values, whereas the isotropic A values for Cu(acac)$_2$ and CuTPP estimated with Local and gradient corrected functionals PWP and Ahlrichs basis set DZ agree well with the experimental values.

8:12AM H40.00002 Application of Bayesian Inference and Relativistic Density Functional Theory on EPR Study of Biologically important Transition Metal (Vanadium) Compounds, INDIRA SAHU, LAXMAN MAINALI, KEITH EARLE, SUNY Albany — Quantitative lineshape analysis based on the stochastic Liouville equation allows one to infer information about spin probe structure and dynamics. The EPR parameters extracted from Experimental spectra can be used to check theoretical calculation based on Relativistic Density Functional Theory. Experiments on Vanadyl acetylacetonate [VO(acac)$_2$] and Vanadyl mesotetraphenyl porphine [VO(TPP)] in toluene at different temperatures were performed at five different frequencies(S,X,K,Q & W-band). Spectral Analysis was performed using methods of Bayesian Inference at the various frequencies, both independently and in a simultaneous multifrequency fit. Rotational diffusion parameters were inferred for two symmetries (Axial and Rhombic). The isotropic A value (A$_{iso}$) calculated for VO(acac)$_2$ with unrestricted and hybrid-functional PW1PW and for VO (TPP) with unrestricted and hybrid functional BHLYP and Pople style basis set with polarization function 6-311G(3df,3pd), deviated by 0.95% and 0.23% respectively compared to experimental A$_{iso}$ values. The isotopic g values (g$_{iso}$) calculated for VO (acac)$_2$ and VO(TPP) with unrestricted and hybrid-functional PW1PW and Ahlrichs basis set TZV, deviated by 0.18% and 0.05% respectively compared to experimental g$_{iso}$ values.

8:24AM H40.00003 Electrically stimulated contractions of Vorticella convallaria, DEEPENDRA KANTHA, DAVID VAN WINKLE, Department of Physics and Center for Materials Research and Technology (MARTECH), Florida State University — The contraction of Vorticella convallaria was triggered by applying a voltage pulse in its host culturing medium. The 50V, 1ms wide pulse was applied across platinum wires separated by 0.7 cm on a microscope slide. The contractions were recorded as cines (image sequences) by a Phantom V5 camera (Vision Research) on a bright field microscope with 20X objective, with the image size of 256 pixels $\times$ 128 pixels at 7352 pictures per second. The starting time of the cines was synchronized with the starting of the electrical pulse. We recorded five contractions of each of 12 organisms. The cines were analyzed to obtain the initiation time, defined as the difference in time between the leading edge of the electrical pulse and the first frame showing zoid movement. From multiple contractions of the same organism, we found the initiation time is reproducible. In comparing different organisms, we found the average initiation time of 1.73 ms with a standard deviation of 0.63 ms. This research is supported by the state of Florida (MARTECH) and Research Corporation.

8:36AM H40.00004 Pressure Effects on the Morphology of Mammalian Cells, JOHN SCHROEDER, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180, CHARLES R. KEESE, Appliedbiophysics Inc., 185 Jordan Rd., Troy, NY 1218010var, IVAR GIAEVER, Applied Biophysics Inc, 185 Jordan RD Try, NY 12180 — Living mammalian cells can be perturbed by high pressure in a continuous and controlled manner. The effects can be easily measured and quantified using the well-established method of Electric Cell-substrate Impedance Sensing (ECIS). ECIS is an electrical biosensor that quantitatively monitors behaviours of living cells including spreading and adhesion, micromotion and migration. Here we describe the experimental set-up of the pressure equipment and how ECIS is adapted to data collection under these conditions. Preliminary results suggest that high pressure affects the cell attachment and spreading and causes well-attached cells to round up. Results will be presented on the behavior of monolayers of BSC-1 cells upon application of pressures up to 2 kbars of nitrogen gas.

8:48AM H40.00005 The electronic properties of microbial nanowires: An STM investigation, JOSH VEAZEY, BECKY STEIDL, GEMMA REGUERA, STUART TESSMER — Geobacter species of bacteria present the prospect of an interesting physical system through the expression of pili that act as electrically conductive nanowires. These nanowires serve the biological role of transporting metabolically generated electrons outside the cell body to electron acceptors in the organism’s native environment. We have performed scanning tunneling microscopy and spectroscopy on Geobacter sulfurreducens in an effort to elucidate the mechanism of conductivity. Understanding this system may lead to the enhancement in the effectiveness of Geobacter species’ roles in microbial fuel cells and the bioremediation of hazardous waste, such as uranium and petroleum.

9:00AM H40.00006 Probing Ion Channel Insertion into a Bilipid Membranes with a Radio Frequency Tank Circuit, HYUN CHEOL SHIN, Materials Science Program, University of Wisconsin-Madison, WI 53706, ERIC STAFA, MINRUI YU, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706, HUA QIN, Suzhou Institute of Nano-Tech and Nano-Bionics, Suzhou City, Jiangsu 215123, People’s Republic of China, HYUN-SEOK KIM, ROBERT BLICK, Department of Electrical and Computer Engineering, University of Wisconsin-Madison, WI 53706 — We fabricated a radio frequency resonant circuit which can be applied for probing ion channels formed in bilipid membranes. The insertion of ion channels can be probed by monitoring the resonant response of the tank circuit. The circuit itself is realized on a glass chip, which simultaneously uses DC channel recordings (i.e. conventional on-chip patch clamping) and RF detection. The direct current recordings of the ion channels responses allows for the calibration of the radio frequency signal. Such radio frequency recordings of ion channel activity have great potential for high-throughput drug screening.

9:12AM H40.00007 Highly oil-producing microalgae selected through directed-evolution on a microfluidic chip, TROY MESTLER, ANDRE ESTEVEZ-TORRES, GUILLAUME LAMBERT, ROBERT H. AUSTIN, Princeton University — Some species of photosynthetic microalgae produce significant amounts of oil which can be easily converted to diesel fuel. However, as it stands today, biodiesel is significantly more expensive than fossil fuels. We wish to improve the oil yield and production rate of a single species of microalgae through directed evolution. We propose to utilize our microfabrication technology to create microhabitats to control the nutrient environment of the species, monitor oil production through Raman Spectroscopy, and punish colonies of algae which have low oil yield. We believe this process will produce a mutant species with a high oil yield.
9:24AM H40.00008 Structural Color of Biological and Biomimetic Amorphous Nanostructures, JASON FORSTER, HEESO NOH, VINODKUMAR SARANATHAN, HUI CAO, SIMON MOCHRIE, CHINEDUM OSUJI, RICHARD PRUM, ERIC DUFRESNE, Yale University — The feathers of many bird species have amorphous nanostructures of beta-keratin and air that produce non-iridescent color. These structural colors are the result of wavelength-selective scattering from nanostructures which have well-defined length scales but no long-range translational order. We quantify the optical properties of feathers with angle-resolved reflectance spectra and compare them to the nanostructure observed with X-ray scattering. We are exploiting self-assembly of polymeric and colloidal systems to create biomimetic nanostructures that capture the essential optical properties of bird feathers. By varying the characteristic length scale and index of refraction contrast of these structures we aim to enhance and tune wavelength selectivity.

9:36AM H40.00009 Directed Fluid Transport and Mixing with Biomimetic Cilia Arrays, A.R. SHIELDS, University of North Carolina - Chapel Hill, B.K. EVANS, Eric University, B.L. CARSTENS, M.R. FALVO, S. WASHBURN, R. SUPERFINE, University of North Carolina - Chapel Hill — We present results on the long-range, directed fluid transport and fluidic mixing produced by the collective beating of arrays of biomimetic cilia. These artificial cilia are arrays of free-standing nanorods roughly the size of biological cilia, which we fabricate from a polymer-magnetic nanoparticle composite that can be moved on a nanometer scale and actuated with permanent magnets to mimic biological cilia. The artificial cilia are modeled to produce low Reynolds number fluid transport and are increasingly being recognized as critical components in a wide range of biological systems. However, despite much effort cilia generated fluid flows remain an area of active study. In the last decade, cilia-driven fluid flow in the embryonic node of vertebrates has been implicated as the initial left-right symmetry breaking event in these embryos. With silica we generate directional fluid transport by mimicking the tilted conical beating of these nodal cilia. By seeding fluorescent microparticles into the fluid we have noted the existence of two distinct flow regimes. The fluid flow is directional and coherent above the cilia tips, while between the cilia tips and the floor particle motion is complicated and suggestive of chaotic advection.

9:48AM H40.00010 Physics of phagocytosis of foreign versus self-tolerance, RICHARD TSAI, PIA RO-DRIGUEZ, DENNIS DISCHER, University of Pennsylvania — The first cells to ‘attack’ an implanted or injected foreign material or microbe are phagocytic cells of the innate immune system. These cells actively and rapidly phagocytose foreign cells, surfaces, or particles, but the process is inefficient when faced with “self” cells. We have examined the biochemistry and some of the physics of this decision to eat or not eat. One particular protein on all animal cell membranes, called CD47, seems to engage phagocytic cell counter-receptors, and deactivate the force-generating myosin machinery that otherwise makes phagocytosis efficient. We will map the phagocytic synapse between phagocytes and particles or cells and describe the physicochemical dynamics that mediate this key decision in compatibility.

10:00AM H40.00011 The Dynamics of Foraging Ants, G. WILLIAM BAXTER, Penn State Erie, The Behrend College — We experimentally study the foraging of small black ants, Formicinae lasius fulvus, in order to describe their foraging behavior mathematically. Individual ants are allowed to forage on a two-dimensional surface in the absence of any food sources. The position of the ant as a function of time is determined using a high-resolution digital camera. Analysis of the average square displacements of many ants suggests that the foraging strategy is a non-reversing random walk. Moreover, the ants do not retrace their steps to return home but instead continue the random walk until it brings them back near their starting point.

10:12AM H40.00012 Elasticity in Ionically Cross-Linked Neurofilament Networks, NORMAN YAO, YI-CHIA LIN, Harvard University Department of Physics, CHASE BROÖDERSZ, Vrije University, KAREN KASZA, Harvard University SEAS, FREDERICK MACKINTOSH, Vrije University, DAVID WEITZ, Harvard University Department of Physics and SEAS — Neurofilaments are found in abundance in the cytoskeleton of nerve cells and they experience mechanical forces from extracellular stresses. To elucidate the nature of the mechanical properties that provide this protection, we measure the linear and nonlinear viscoelastic properties of networks of neurofilaments. These networks are soft solids that exhibit dramatic strain stiffening above critical strain ranges of 30-70%. Surprisingly, divalent ions, such as Mg$^{2+}$, Ca$^{2+}$, and Zn$^{2+}$, act as effective cross-linkers for neurofilament networks, controlling their solid-like elastic response. This behavior is comparable to that of actin-binding proteins in reconstituted filamentous actin. We show that the elasticity of neurofilament networks is entropic in origin and is consistent with a model for cross-linked semiflexible networks, which we use to quantitatively model cross-linking networks. Ultimately, we are able to extract microstructural network parameters such as the persistence length and the average distance between cross-links directly from bulk rheology.

10:24AM H40.00013 Exploring Cell-Assisted Cell Growth, ELLIJA BOGART, SHARON LAU, AMRISH DESHMUKH, CARL FRANCK, Cornell University — The population dynamics of microbial life in sheared liquid suspension affords opportunities to explore the ways in which cells can use each other to proliferate. Such elegant systems continue to inspire us to develop and test simple theories for cooperative behavior (e.g. Phys. Rev. E v. 77, p. 041905 (2008)) in living matter. We report on new insight afforded by the observation of the amoebae Dictostelium discoideum of the effect of population growth of the introduction of adhesive contacts of cells with each other as well as solid substrates. Through a hydrodynamic scaling argument we find that mechanical triggers provided by intercellular collisions are more important than collisions with container walls in encouraging growth. Finally, we confirm the discovery of a strain that lacks growth regulation due to density sensing. This work was supported by the NIH (P01 GM07856).

10:36AM H40.00014 Small Molecules Target Carcinogenic Proteins, CLAUDIU GRADINARU, University of Toronto — An ingenious cellular mechanism of effecting protein localization is prenylation: the covalent attachment of a hydrophobic prenyl group to a protein that facilitates protein association with cell membranes. Fluorescence microscopy was used to investigate whether the oncogenic Stat3 protein can undergo artificial prenylation via high-affinity prenylated small-molecule binding agents and thus be rendered inactive by localization at the plasma membrane instead of nucleus. The same approach was performed on a biological framework protecting the neuron from extracellular stresses. To elucidate the nature of the mechanical properties that provide this protection, we measure the linear and nonlinear viscoelastic properties of networks of neurofilaments. These networks are soft solids that exhibit dramatic strain stiffening above critical strain ranges of 30-70%. Surprisingly, divalent ions, such as Mg$^{2+}$, Ca$^{2+}$, and Zn$^{2+}$, act as effective cross-linkers for neurofilament networks, controlling their solid-like elastic response. This behavior is comparable to that of actin-binding proteins in reconstituted filamentous actin. We show that the elasticity of neurofilament networks is entropic in origin and is consistent with a model for cross-linked semiflexible networks, which we use to quantitively model cross-linking networks. Ultimately, we are able to extract microstructural network parameters such as the persistence length and the average distance between cross-links directly from bulk rheology.

10:48AM H40.00015 Direct observation of DNA dynamics toward solid state nanopore studied by fluorescence microscopy, TOMOHARU TAKITA, NORIYUKI TOYAMA, KAYA KOBAYASHI, TOSHIYUKI MITSU, Aoyama-Gakuin University — Translocation of single DNA through a solid state nanopore provides information of the length and the folding configuration of the DNA by sensing the ionic current profile. This sensing method opens the possibility to characterize individual polynucleotide molecule such as DNA and RNA and their interaction with various proteins. The interesting phenomena related to the nanopore based DNA sensing with the translocating ionic current have been reported recently and we also have found unexpected clogging probability of DNA into pore as a function of the biased voltage across the pore membrane. To visualize these phenomena as the dynamics of individual DNA molecule near nanopore, we have used fluorescence microscopy. The acceleration of DNA caused by an attractive force toward nanopore was observed in sequential images of the microscope images. By applying the langevin equations to follow the dynamical motion of DNA, the electric fields near the nanopore under the various biased voltages and ionic concentrations were estimated in DNA solution. In this presentation, we will report the results of the estimated electric fields near nanopore and discuss the shape of the potential.
8:00AM H41.00001 X-ray Diffraction measurements of the CDW phase in doped TiSe₂ and NbSe₂ , J.P. CASTELLAN, Argonne Nat. Lab, C.D. MALLIAKAS, Northwestern University, M. LAVARONE, S. ROSENKRAZ, Argonne Nat. Lab., R. OSBORN, Argonne Nat. Lab., F. WEBER, Argonne Nat. Lab. — Layered transition metal chalcogenides display a phase diagram similar to that of high Tc superconducting materials. In high Tc materials the superconductivity coincides with the suppression of magnetic order. In the case of TiSe₂ and NbSe₂ the onset of superconductivity involves a charge density wave (CDW) rather than magnetic order. The phase diagram of doped TiSe₂ and NbSe₂ has so far been interpreted as a competition of the CDW order and superconductivity order parameters. Another interpretation is that the softening of the excitons responsible for the CDW order enables the superconductivity. We have measured diffuse scattering associated with the fluctuations in the order parameter of the CDW on either side of the quantum phase transition using X-ray scattering. We will present the behavior of the critical exponents as the quantum phase transition is approached and discuss whether there is a coupling of the CDW and superconducting order parameters. Work supported by US DOE BES-DMS DE-AC02-06CH11357

8:12AM H41.00002 Interplane and Intraplane Coupling in Charge-Density-Wave Phases of 1T-TaS₂ and 1T-TaSe₂ , YIZHI GE, AMY LIU, Georgetown University — At low temperatures, the layered transition metal dichalcogenides 1T-TaS₂ and 1T-TaSe₂ adopt similar charge-density wave structures corresponding to a √3 x √3 reconstruction in which the Ta atoms cluster within the triangular layers. Yet TaS₂ also undergoes a metal-insulator transition, while TaSe₂ does not. Here we present a density-functional-theory study of the electronic structure of 1T-TaS₂ and 1T-TaSe₂. The half filled Ta d band at the Fermi level is found to differ significantly in the two materials: in TaSe₂ the band is three dimensional, while in TaS₂ it is highly one dimensional. These results are analyzed using maximally localized Wannier functions. The effects of stacking sequence and the spin-orbit interaction will also be discussed.

8:24AM H41.00003 A time-resolved observation of collective phenomena in the CDW compound TbTe₃ , F. SCHMITT, Stanford University, P. S. KIRCHMANN, U. BOVENSIEPEN, F. U. Berlin, R. G. MOORE, SRL, L. RETTIG, M. KRENZ, F. U. Berlin, J.-H. CHU, N. RU, Stanford University, L. PERFETTI, F. U. Berlin, D.-H. LIU, SRL, M. WOLF, F. U. Berlin, I. FISHER, Z.-X. SHEN, Stanford University — Strong correlations and collective phenomena in solids are a fascinating and challenging area of physics. Understanding how the interactions between the constituents give rise to collective phenomena like phase transitions and collective modes will greatly enhance our understanding in solid state physics. One such system, the Rare Earth TlTetrilulrides RT₆₃, is an excellent model system for a systematic study of charge-density wave (CDW) physics. We have performed time-resolved angle-resolved photoelectron spectroscopy (trARPES), a novel form of pump-probe spectroscopy, on Tb₆₃ and we will present our newest results. We observe two collective modes and what we term the time-dependent melting of the CDW, which we discussed earlier. Here, we will focus primarily on the detailed properties of the two collective modes.

1Supported by DFG and DOE
3This research was supported by NSF-DMR Grants 0801764 and 0400938.

8:36AM H41.00004 Voltage Induced Torsional Strain in Tantalum Trisulfide in its CDW State , J. NICHOLS, JUN ZHOU, L. LADINO, J.W. BRILL, University of Kentucky — In 2007, Pokrovskii et al [Phys. Rev. Lett. 98, 206404 (2007)] reported that crystals of tantalum trisulfide spontaneously twist when a voltage near the CDW depinning threshold is applied. The direction of twist reverses when the voltage is reversed, so that the twist angle describes a characteristic hysteresis loop as a function of applied voltage or current. We have studied this effect by placing the sample inside a resonant RF cavity so that the twisting sample modulates the resonant frequency of the cavity. A magnetic wire is attached to the sample so that magnetic torque can also be applied to the sample. We have reproduced the "Pokrovskii effect" and also observed the complement: application of torque induces an additional strain when the sample is biased above threshold. We have also found that the onset of the torsional strain occurs at a voltage slightly below that at which the shear modulus of the sample softens.

8:48AM H41.00005 Evidence for coupling between charge-density-wave and phonons in two-dimensional rare-earth tri-tellurides , M. LAVAGNINI, ETH-Zurich, M. BALDINI, La Sapienza Rome, A. SACCHETTI, ETH-Zurich, D. DI CASTRO, La Sapienza Rome, B. DELLEY, PSI Villigen, R. MONNIER, ETH-Zurich, J.H. CHU, N. RU, I.R. FISHER, Stanford University, P. POSTORINO, La Sapienza Rome, L. DEGIOGRI, ETH-Zurich — We report on a Raman scattering investigation of the charge-density-wave (CDW), quasi two-dimensional rare-earth tri-tellurides RT₆₃ (R=Ta, Ce, Pr, Nd, Sm, Gd and Dy) at ambient pressure, and of LaTe₃ and CeTe₃ under externally applied pressure. The observed phonon peaks can be ascribed to the Raman active modes for both the undistorted as well as the distorted lattice in the CDW state by means of a first principles calculation. The latter also predicts the Kohn anomaly in the phonon dispersion, driving the CDW transition. The integrated intensity of the two prominent modes scales as a characteristic power of the CDW-gap amplitude upon compressing the lattice, which provides clear evidence for the tight coupling between the CDW condensate and the vibrational modes.

9:00AM H41.00006 Pressure dependence of the single particle excitation in the charge-density-wave CeTe₃ system , L. DEGIOGRI, M. LAVAGNINI, A. SACCHETTI, ETH-Zurich, C. MARINI, M. VALENTINI, R. SOPRACASE, A. PERUCCHI, P. POSTORINO, S. LUPI, La Sapienza Rome, J.H. CHU, I.R. FISHER, Stanford University — We present data on the pressure dependence at 300 K of the optical reflectivity of CeTe₃, which undergoes a charge-density-wave (CDW) phase transition well above room temperature. The collected data cover an unprecedented broad spectral range from the infrared up to the ultraviolet, which allows a robust determination of the gap as well as of the fraction of the Fermi surface affected by the formation of the CDW condensate. Upon compressing the lattice there is a progressive closing of the gap inducing a transfer of spectral weight from the gap feature into the Drude component. At frequencies above the CDW gap we also identify a power-law behavior, consistent with findings along the RT₆₃ series (i.e., chemical pressure) and suggestive of a Tomonaga-Luttinger liquid scenario at high energy scales.
9:12AM H41.00007 Far infrared magnetospectroscopy of quasi-1D and 2-D density wave compounds,1 A.F. ISAKOVIC, G.L. CARR, NSLS, Brookhaven National Lab — We report a far infrared reflectance study of quasi-1D blue bronze (K1.3MoO3)2 and magnetically doped quasi-2D Mn611–xBa11xBi2223 over the temperature range from 10K up to 180K and fields up to 10T. For blue bronze, several features in the magnetoreflectance spectra, including amplitude and phonon-like modes, change substantially (up to 50%) when a magnetic field is applied. For 100K< <180K (below the CDW Tc of 183K), the spectra change nearly monotonically with T. Changes at lower T involve primarily the amplitude mode (CDW order parameter), consistent with creep transport of the CDW. The B and T dependent spectra of Mn doped NbSe2 reveal the presence of an isosbestic point near 5 meV photon energy and having a shape suggesting a local transfer of oscillator strength. The magnetoreflectance changes abruptly around a temperature of 16K for fields below 6T. Though a Drude-Lorentz fit can be applied to the spectra, a full understanding of charge transport in these materials will require a more detailed model.

1Supported by DOE (DE-AC02-98CH10886) and NSF. Use of R.P. Thorne lab (Cornell Univ.) for sample preparation and the CCNY high-field magnet (J.J. Tu) are gratefully acknowledged.

9:24AM H41.00008 Microwave dielectric study of spin-Peierls and charge ordering transitions in (TMTTF)2PF6 salts, MARIO PORIER, ALEXANDRE LANGLOIS, CLAUDE BOURBOUNNAIS, Universite de Sherbrooke, PASCALE FOURY-LEYLEKIAN, ALEC MORAPOUR, Universite Paris XI Orsay — Using a microwave cavity perturbation technique at 16.5 GHz, we report a temperature and magnetic field study of the complex dielectric function along the stacking a-axis for a (TMTTF)2PF6, single crystal and its deuterated analog (d12). For both salts, the charge ordering transition (CO) is characterized by a decrease of the dielectric constant εa centered at TC0 (65 K and 85 K); concomitantly, the dielectric losses go through a maximum near TC0 and decreases rapidly below. The spin-Peierls transition (SP) is rather signalled by a rapid increase of εa below TSP (16 K and K3 K) accompanied by a small peak in the losses. For the deuterated salt, we have observed important relaxation effects below 40 K that complicate the analysis of the dielectric function in the SP ground state. The temperature dependence of the SP anomalies was analysed in magnetic field values up to 18 Tesla.

9:36AM H41.00009 NMR spin echo measurements of sliding spin density wave repinning in (TMTSF)2SbF6, W.G. CLARK, UCLA Physics and Astronomy, M.E. HANSON, SAP Labs, LLC., ERNEST W.H. WONG, Varian Inc. — We report the repinning rate of sliding spin density waves (SDW’s) in (TMTSF)2PF6, obtained from proton spin echo measurements. This method provides a local measurement of the square of the magnitude of the SDW velocity averaged over the sample as a function of time after the electric field responsible for the SDW sliding is reduced to below its depinning value. It shows a slow decay of the SDW current which we attribute to the corresponding adjustment of the SDW phase to the pinning centers and relaxation of the strain of the sliding SDW. Above the temperature T ~4 K, a thermally activated behavior for the characteristic decay time is observed whose activation energy of 2±1 K is close to the single electron excitation gap. This indicates that above 4 K, the repinning rate is dominated by thermally excited electrons. Below 4 K, a much weaker T-dependence is observed suggesting that tunneling may become the dominant repinning mechanism at lower T.

1This work was supported in part by NSF Grants DMR-9705369 and 0334809.

9:48AM H41.00010 Low-temperature states in quasi-one-dimensional charge transfer salt (TMTSF)2SbF6 studied by 13C NMR under hydrostatic high pressures, FUMITATSU IWASE, Institute for Molecular Science, KOICHI SUGIURA, The Graduate University for Advanced Studies, KOU FURUKAWA, TOSHIKAZU NAKAMURA, Institute for Molecular Science — We report 13C NMR study of a quasi-one-dimensional charge transfer salt, (TMTSF)2SbF6, under the application of the hydrostatic pressure. The antiferromagnetic phase transition at ambient pressure was confirmed by the line splitting and the divergent increase of the spin-lattice relaxation rate 1/T1. Under ~5 kbar, 1/T1 decreases abruptly at low temperatures without the enhancement, indicating that the ground state is a spin-gapped phase. However, the decrease of the Knight shift expected for spin-Peierls phase transition has not been observed. We observed additional lines, which split symmetrically, at low T, possibly originating from other states.

10:00AM H41.00011 The Theory of the Field-Induced Charge-Density-Wave Phases,1 ANDREI LELED, Dept. of Physics, University of Arizona — We study a problem about the appearance of the Field-Induced Charge-Density-Wave (FICDW) phases in a quasi-one-dimensional conductor in high magnetic fields. The calculated ratios for critical magnetic fields of the different FICDW phase transitions are in very good agreement with the existing experimental data in alpha-(ET)2K(Hg(SCN)4).

1This work was supported by the NSF grant DMR-0705986.

10:12AM H41.00012 Realistic Parameters for the Description of Organic Metals, ANDREAS DOLFEN, German Research School for Simulation Sciences, Germany, ERIK KOCH, Institut für Festkörperforschung, Forschungszentrum Jülich, Germany, VOLKER BLUM, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, LAURA CANO-CORTES, JAIME MERINO, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain — In molecular crystals correlation effects are often significant. For a non-perturbative description of the full Coulomb interaction we have therefore to resort to a model description in terms of generalized Hubbard models. The derivation of parameters for such models is crucial for realistic simulations. While hopping parameters are easily derived from density-functional theory (DFT) the Coulomb parameters pose a significant problem due to screening processes. We decompose their contributions into intra- and inter-molecular parts. The intra-molecularly screened parameters are realistic and the distributed-dipole approach in combination with a Ewald summation. Even for simple lattices of polarizable point dipoles we find intriguing screening phenomena. As realistic applications we discuss the one- and two-dimensional organic metals TTF-TCNO and θ-(BEDT-TTF)2I3.

10:24AM H41.00013 Spinodal decomposition of the charge ordering in the θ-based organic salt, MAJED ABDDEL-JAWAD, ICHIRO TERASAKI, Waseda University, HATSUMI MORI, University of Tokyo, TAKEHIKO MORI, Tokyo Institute of Technology — We have measured with X-ray diffraction, resistivity and thermopower the spinodal decomposition of the long range charge ordering in the organic compounds θ-(BEDT-TTF)2RbZn(SCN)4 and θ-(BEDT-TTF)2RbCo(SCN)4. Details of this spinodal decomposition reveals that the charge ordering growth in these compounds follows at first a two dimensional diffusion controlled mode followed abruptly by a change to a three dimensional diffusion controlled growth. Thermopower reveals that the long ranged charge ordered state in these compounds is characteristic of a system with strong on-site repulsion with narrow bandwidths. In contrast to this, the thermopower of the short ranged charge ordering is anomalous not only in its value but also in its temperature dependence.
are either not exactly coplanar with graphene, or are correlated, or are not the only source of disorder. This work is supported by the NSF.

dielectric-constant environment where Coulomb interactions of electrons with impurities and electrons with each other become weak. We show that screening

solution of the model of graphene subject to the disorder in the form of in-plane charged impurities. Our approach is asymptotically exact for graphene in high

nature of disorder at the NP and the still unsettled question of which type of disorder is really dominant. Here, we report on our progress towards analytical

socalled $\rho_{xx}(\theta, \phi)$ of the layered organic conductor (DMET)$_2$I$_3$ is reported for all possible orientations in a 9T magnetic field at 100 mK, and compared with existing theoretical models. We have also calculated $\rho_{x}\perp$ for such Q1D conductors using semiclassical calculations employing, for the first time, the true triclinic crystal structure. These calculations are in qualitative agreement with our data, especially in the $\gamma - z$ plane, where all previous models fail to reproduce the experimentally observed Lebed magic angle effect. These results will be useful to understand the relationship between the different kinds of angular effects in this and other families of layered organic conductors. This work was supported by NSF Grant No. DMR 0605339. [1]. H. Yoshino, et al., (unpublished). [2]. S. Uji, et al., Proceeding of Physical Phenomena at High Magnetic Fields III (World Scientific, London, 1998), p 227. [3]. A. G. Lebed, JETP Lett. 43, 174 (1986); T. Osada, et al., Phys. Rev. Lett. 66, 1525 (1991); M. J. Naughton, et al., Phys. Rev. Lett. 67, 3712 (1991).

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J1 DCMP: Ballistic-Diffusive Crossover in Graphene Electron Transport
Spirit of Pittsburgh Ballroom A

11:15AM J1.00001 Electrical transport in suspended graphene, KIRILL BOLOTIN, Columbia University — Many quantum limit transport phenomena in graphene remain yet to be observed due to the omnipresence of carrier scattering. We report a sample preparation method that yields high quality graphene specimens and demonstrates that much of the scattering in traditional graphene-on-silica devices is not intrinsic but rather results from the interaction with the substrate underlying the graphene. We fabricate devices where electrically contacted and electrostatically gated graphene flakes are suspended over a substrate and use current-induced heating to remove the remaining impurities. The measured mobilities are found to exceed 200,000 cm$^2$/Vs in such devices, an order of magnitude improvement over the best values reported in the literature. The very high mobility of our specimens allows us to probe previously inaccessible transport regimes in graphene. At low temperatures transport is near-ballistic in a device of $\sim$2µm dimension. At large carrier density, we observe linear increase of resistivity with temperature, consistent with scattering off acoustic phonons. At near-room temperature we observe the mobility is $\sim$120,000 cm$^2$/Vs, higher than in any known semiconductor.

11:51AM J1.00002 A self-consistent theory for graphene transport, SHAFFIQUE ADAM, University of Maryland — Arguably, one of the most intriguing properties of graphene transport is the non-vanishing “minimum conductivity” at the Dirac point. The carrier density in these single monatomic sheets of carbon can be continuously tuned from electron-like carriers for large positive gate bias to hole-like carriers for negative bias. The physics close to zero carrier density (also called the intrinsic or Dirac region), is now understood to be dominated by the inhomogeneous situation where the local potential fluctuates around zero, breaking the landscape into puddles of electrons and holes. Here, we propose and discuss a particular hierarchy of approximations to understand graphene transport properties that includes a tight binding approximation for the low energy effective Hamiltonian, Random-Phase-Approximation to treat electron-electron interactions, the semi-classical Boltzmann transport theory to treat scattering of electrons by short and long-ranged disorder, and a self-consistent Fermi-Thomas approximation to treat impurity induced density inhomogeneity [1-2]. We find that this self-consistent theory for graphene transport is in remarkable agreement with recent experiments [3-5]. To better understand the range of validity of this theory we relax some of the assumptions and include the effects of tunneling [6], calculate transport properties using an effective medium theory [7], and examine the effects of phase-coherent quantum transport [8]. We believe that while most of the dc transport experiments on bulk graphene samples at zero magnetic field are in the parameter regime correctly captured by the semi-classical diffusive self-consistent transport theory, we demonstrate theoretically that by tuning external parameters, it is possible to access several other transport regimes.

References:
[2] Hwang, Adam, and Das Sarma, PRL 98, 186806 (2007);

This work is supported by US-ONR and NRI-SWAN and done in collaboration with Sankar Das Sarma, Michael Fuhrer, Euyheon Hwang, Victor Galitski, Piet Brouwer, and Enrico Rossi.

12:27PM J1.00003 Theory of an inhomogeneous electron structure of graphene at its neutrality point, MICHAEL FOLGER, University of California, San Diego — Graphene is a surprisingly good conductor. Despite its direct exposure to various sources of disorder (charged impurities, non-uniformity of the substrate, etc.), graphene remains conductive even when the nominal concentration of both electron and hole carriers drops to zero - the neutrality point (NP). Theory of the minimal conductivity of graphene is an outstanding challenge because of the non-perturbative nature of disorder at the NP and the still unsettled question of which type of disorder is really dominant. Here, we report on our progress towards analytical solution of the model of graphene subject to the disorder in the form of in-plane charged impurities. Our approach is asymptotically exact for graphene in high dielectric-constant environment where Coulomb interactions of electrons with impurities and electrons with each other become weak. We show that screening of the impurity potential is nonlinear, producing a fractal structure of electron and hole puddles. Statistical properties of this density distribution as well as the charge compressibility of the system are calculated in the leading-log approximation. The minimal conductivity is shown to depend logarithmically on the dielectric constant. We compare our results with other theoretical works and current experiments. Our findings suggest that in real samples charged impurities are either not exactly coplanar with graphene, or are correlated, or are not the only source of disorder. This work is supported by the NSF.
1:03PM J1.00004 Electronic Transport in Disordered Graphene Sheets and Nanoribbons
EDUARDO R. MUCCIOLO, University of Central Florida — In this talk I will present recent results of our numerical simulations of electronic transport in disordered graphene. Issues related to the scaling of the conductivity and the shot-noise Fano factor of large graphene sheets at zero and finite doping will be discussed. Our calculations are based on an efficient implementation of the recursive Green function method. I will also show how edge and bulk disorder may affect the mesoscopic conductance of graphene nanoribbons under a variety of realistic situations. We find that even for weak edge roughness, conductance steps are suppressed and a transport gap develops near the neutrality point due to strong localization. The gap inferred from our simulations is similar in magnitude to the energy gaps induced by other mechanisms, such as Coulomb blockade, multi-body correlations, and lattice distortions. The effects of dephasing will also be discussed.

1:39PM J1.00005 Electron fractionalization in two-dimensional graphenelike structures CLAUDIO CHAMON, Boston University — Electron fractionalization is intimately related to topology. In one-dimensional systems, such as polycatenane, fractionally charged states exist at domain walls between degenerate vacua. In two-dimensional systems, fractionalization exists in quantum Hall fluids, where time-reversal symmetry is broken by a large external magnetic field. Recently, there has been a tremendous effort in the search for examples of fractionalization in two-dimensional systems with time-reversal symmetry. Here we show that fractionally charged topological excitations exist in tight-binding systems where time-reversal symmetry is respected. These systems are described, in the continuum approximation, by the Dirac equation in two space dimensions. The topological zero-modes are mathematically similar to fractional vortices in p-wave superconductors. They correspond to a twist in the phase in the mass of the Dirac fermions, akin to cosmic strings in particle physics. The quasiparticle excitations can carry irrational charge and irrational exchange statistics. These excitations can be deconfined at zero temperature, but when they are, the charge re-rationalizes to the value 1/2. REFS.: Chang-Yu Hou, Claudio Chamon, Christopher Mudry, Phys. Rev. Lett. 98, 186809 (2007); Claudio Chamon, Chang-Yu Hou, Roman Jackiw, Christopher Mudry, So-Young Pi, Andreas P. Schnyder, Phys. Rev. Lett. 100, 110405 (2008); Claudio Chamon, Chang-Yu Hou, Roman Jackiw, Christopher Mudry, So-Young Pi, Gordon Semenoff, Phys. Rev. B 77, 235431 (2008)

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J2 DCMP: Dynamical Layer Decoupling and Stripe Order High Tc Superconductors
Spirit of Pittsburgh Ballroom BC

11:15AM J2.00001 Towards two-dimensional superconductivity in La_{2-x}Sr_{x}CuO_{4} in a moderate magnetic field^1 ALEXANDER SCHAFFGANS, Department of Physics, University of California, San Diego — We report a novel aspect of the competition and coexistence between antiferromagnetism and superconductivity in the prototypical high-Tc cuprate La_{2-x}Sr_{x}CuO_{4} (La214). With a modest magnetic field applied H || c-axis, we monitored the infrared signature of pair tunneling between the CuO2 planes and discovered the complete suppression of interlayer coupling in a series of La214 single crystals. We find that the in-plane superconducting properties remain largely intact, in spite of increased antiferromagnetism in the planes. Thus, our experiments show that an isolated CuO2 plane is capable of maintaining high-Tc superconductivity. The theoretical framework for antiferromagnetic-driven interlayer decoupling is identified in the work of Berg, et. al. [E. Berg, et. al., Phys. Rev. Lett. 99, 127003 (2007) and Cond-mat arXiv:0810.1564].

^1Work at UCSD is supported by the National Science Foundation (NSF-DMR-0705171)

11:51AM J2.00002 Theory of a striped superconductor ERZE BERG, Stanford — In the spin and charge striped-ordered cuprate La_{1-x}Ba_{x}CuO_{4}, the bulk superconducting Tc is strongly suppressed to about 4K. Nevertheless, recent experiments revealed unusual superconducting fluctuations far above Tc. In particular, these experiments show evidence for 2D superconductivity in this 3D (albeit anisotropic) system, which is unprecedented. We propose an explanation of these results in terms of a new phase, the “striped superconductor”, in which the superconducting order parameter is modulated periodically in space and averages to zero. Such a state can naturally explain the apparent vanishing of the inter-layer Josephson coupling in La_{1-x}Ba_{x}CuO_{4}. We discuss several phenomenological features of this phase, including a unique sensitivity to disorder which can lead to an “xy gauge glass” phase that breaks time reversal symmetry spontaneously. Possible microscopic mechanisms leading to striped superconductivity will be briefly discussed.

12:27PM J2.00003 Electronic liquid-crystal phases, symmetry breaking and Fermi-surface reconstruction in YBa_{2}Cu_{3}O_{6+x}^1 VLADIMIR HINKOV, Max-Planck-Institute for Solid-State Research, Stuttgart, Germany — The physics of undoped cuprates is governed by strong correlations and phase competition, and its understanding remains one of the challenges of condensed-matter research. Here we will discuss our systematic doping- and temperature-dependent neutron-scattering investigation of the spin correlations in underdoped YBa_{2}Cu_{3}O_{6+x} (YBCO) in the context of various proposed symmetry-breaking phases. In YBCO6.45 (Tc = 35 K), we observe the spontaneous onset of a one-dimensional, incommensurate (IC) modulation of the low-energy (< 10 meV) spin excitations below T ≈ 150 K, Hinkov et al., Science 319, 597 (2008). We interpret our finding as the occurrence of an electronic liquid-crystal phase breaking C4 symmetry, as predicted by Kivelson et al., Nature 393, 550 (1998). Below T ≈ 30 K, we observe the onset of quasi-static spin-correlations with the same IC geometry as the low-energy spin excitations. Their intensity is doubled by the application of a magnetic field of 15 T. First of all, this resolves a long-standing discrepancy with the La_{2-x}(Sr,Ba)_{x}CuO_{4} family where field-dependent, IC quasi-static spin correlations were reported before (Lake et al., Nature 415, 299 (2002)). More importantly, our results show how the recently reported quantum oscillations in high magnetic fields in YBa_{2}Cu_{3}O_{6.5} (Doiron-Leyraud et al., Nature 447, 565 (2007)) can be understood in terms of a Fermi-surface reconstruction induced by IC spin modulations. In the lack of experimental evidence for such IC modulations, this mechanism has not been pursued in the past, although it was discussed as a straightforward explanation for Fermi-surface reconstruction. Finally, we will discuss YBCO with a Tc of 10 K. Compared to the previous example, there is an enhancement of the quasi-static spin-correlations. In addition, there is indication for incipient commensurate AF order in reminiscence of the AF parent compound.

^1The author acknowledges collaboration with Daniel Hau and financial support by the German Science Foundation within the consortium FOR538.

1:03PM J2.00004 Stripe order, electron pockets, and Fermi arcs^1 MICHAEL NORMAN, Materials Science Division, Argonne National Laboratory — The recent observation of an electron pocket by quantum oscillation experiments is naturally explained by the presence of magnetic stripe order near 1/8 hole doping in cuprates [1]. A bigger question is how these observations are related to other phenomena in the phase diagram - the pseudogap phase, quantum critical points, and Fermi arcs [2], and the implications this might have for the origin of high temperature superconductivity.


^1Work at Argonne National Laboratory was supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.
1:39PM J2.00005 Magnetic Field and Temperature Dependence of Charge Stripe Order in La2-xBaxCuO4 (x~1/8),1, YOUNG-JUNE KIM, University of Toronto — We report a comprehensive x-ray scattering study of charge stripe ordering in La2-xBaxCuO4 (x~1/8), for which the bulk superconducting Tc is greatly suppressed. We found that the charge order in this sample is described with one-dimensional charge density waves, which have incommensurate wave-vectors (0.23, 0, 0.5) and (0, 0.23, 0.5) respectively on neighboring CuO2 planes. The structural modulation due to the charge stripe order is simply sinusoidal, and no higher harmonics were observed. Just below the structural transition temperature, short-range charge density wave correlation appears, which then develops into a large scale charge ordering around 40 K, close to the spin density wave ordering temperature. However, this charge ordering fails to grow into a true long range order, and its correlation length saturates at ~23 nm, and slightly decreases below about 15 K. In addition, we report our observation of the unusual magnetic field dependence of the charge order correlation length. Specifically, in the superconducting phase the charge order correlation length increases as the magnetic field greater than ~5 T is applied.

1Work supported by Natural Science and Engineering Research Council of Canada and Ontario Ministry of Research and Innovation

Tuesday, March 17, 2009 11:15AM - 2:15PM —

Session J3 DCMP: SQUID Amplifiers: at the Quantum Limit

11:15AM J3.00001 Quantum information processing with the Josephson ring modulator, MICHEL DEVORET, Yale University — No abstract available.

11:51AM J3.00002 Nearly noiseless amplification of microwave signals with a Josephson parametric amplifier, MANUEL CASTELLANOS-BELTRAN, JILLA, NIST and the University of Colorado, and the Department of Physics, University of Colorado, Boulder, Colorado 0309-0440, USA — A degenerate parametric amplifier transforms an incident coherent state by amplifying one of its quadrature components while deamplifying the other. This transformation, when performed by an ideal parametric amplifier, is completely deterministic and reversible; therefore the amplifier in principle can be noiseless. We attempt to realize a noiseless amplifier of this type at microwave frequencies with a Josephson parametric amplifier (JPA). To this end, we have built a superconducting microwave cavity containing many dc-SQUIDs. This arrangement creates a non-linear medium in a cavity and it is closely analogous to an optical parametric amplifier. In my talk, I will describe the current performance of this circuit, where I show I can amplify signals with less added noise than a quantum-limited amplifier that amplifies both quadratures. In addition, the JPA also squeezes the electromagnetic vacuum fluctuations by 10 dB. Finally, I will discuss our effort to put two such amplifiers in series in order to undo the first stage of squeezing with a second stage of amplification, demonstrating that the amplification process is truly reversible.


12:27PM J3.00003 Flux-driven Josephson parametric amplifier, TSUYOSHI YAMAMOTO, NEC Corporation — Degenerate parametric amplifiers are phase sensitive amplifiers, which can in principle amplify one of the two quadratures of a signal without introducing extra noise. Parametric amplifiers based on the nonlinearity of an inductance of a Josephson junction have been studied for a long time. Recently, there has been a renewed interest in parametric amplifiers due in part to the increasing need for quantum-limited amplification in the field of quantum information processing using superconducting circuits. In the present work, we design a novel Josephson parametric amplifier, comprising a superconducting transmission-line resonator terminated by a dc SQUID. Contrary to the previous works, the pump is not used to directly modulate a current through the Josephson junction, but is instead used to modulate a flux through the dc SQUID. Because the dc SQUID determines the boundary condition of the resonator, the flux modulation gives the temporal variation of the resonant frequency, which leads to the parametric amplification of the signal coming into the resonator. The practical advantage of the scheme is, first, that the band center of the signal is widely controllable by a dc flux also applied to the SQUID. Second, as the pump and the signal are applied to different ports and their frequencies are twice different, it is straightforward to separate the output signal from the pump. We have operated such a flux-driven Josephson parametric amplifier at around 10 GHz and characterized its basic properties.

1also at RIKEN and CREST-JST

1:03PM J3.00004 Optimizing the Gain and Noise Temperature of Microstrip SQUID Amplifiers, DARIN KINION, LLNL — Microstrip SQUID amplifiers (MSA) offer near quantum-limited sensitivity and gains greater than 20 db at frequencies around 1 GHz. These properties make them desirable for applications ranging from dark-matter axion detection to dispersive readout of superconducting qubits. The input of the MSA is a microstrip transmission line in the shape of a square spiral coil surrounding the hole in the SQUID washer that serves as the ground plane. Near the fundamental resonance, there is strong flux coupling between the input coil and SQUID. To obtain maximum performance it is necessary to know the complete set of complex scattering parameters. We present measurements of the scattering parameters of MSAs cooled to 4.2 K. The input impedance is found by measuring the reverse scattering parameter (S11) and is described well by a low-loss transmission line model. We map the low-loss transmission line model into an equivalent parallel RLC circuit that accurately predicts the observed gain given by the forward scattering parameter (S21). This information is used to optimize the input and output matching circuitry to achieve optimal noise temperature and gain. We will present results for the gain, dynamic range, linearity and noise temperature of these optimized MSAs at 30-500 mK as a function of frequency and SQUID bias. We will compare the results to the prediction of the circuit model and to the theoretical expectation that the lowest noise temperature occurs off-resonance. This work is in collaboration with John Clarke and a portion of this work was supported by DOE.

1:39PM J3.00005 Lumped-Element DC-SQUID Microwave Amplifier, LAFE SPIETZ, NIST — We report on the development at NIST of microwave amplifiers in the 6-8 GHz frequency range using DC SQUIDs. Our design approach is to use small SQUIDs which can be modeled as lumped element circuits, thus separating the design process for the SQUID from that of the microwave impedance transformers. We present our model and measurements of the impedance, gain and noise temperature of these optimized MSAs at 30-500 mK as a function of frequency and SQUID bias. We will compare the results to the prediction of the circuit model and to the theoretical expectation that the lowest noise temperature occurs off-resonance. This work is in collaboration with John Clarke and a portion of this work was supported by DOE.

Tuesday, March 17, 2009 11:15AM - 2:26PM —

Session J4 CSWP, FIP: Panel Discussion: Around the World in 180 Minutes: Differences and Similarities among Women Physicists
World. KARIMAT EL SAYED, Physics Department, Faculty of Science, Ain-shams University — Until the end of the 19th Century Science was not

available female talent pool. If human society is to benefit to its fullest from various contributions that the field of physics can offer in addressing global issues

Although considerable progress has been made since 2002, it was clear that the global scientific workforce is still under-utilizing a large percentage of the

ICWIP unanimously approved a five-part resolution to IUPAP

recommendations actions to promote the recruitment, retention, and advancement of women in physics and related fields.

1 The Conference was partially supported by NSF (PHY#0824634).

12:10PM J4.00004 Marshak Lectureship Talk: Women in Physics in Egypt and the Arab World. KARIMAT EL SAYED, Physics Department, Faculty of Science, Ain-shams University — Until the end of the 19th Century Science was not classified into different disciplines. The first woman named in the history of science was Merit Ptah (2700 BC) in Egypt's Valley of the Kings. In the new Egypt the first girl's school started in Cairo in 1873 and the first University in 1908. Only a few girls attended the University at that time, mainly studying the humanities. The first Egyptian woman physicist graduated in 1940 and received her PhD in nuclear physics in the USA. Nowadays the number of women in physics is increasing in all branches of physics, some of them are senior managers and others have been decorated with various prizes. In this talk some statistics will be given to show the percentage of women in physics in relation to other fields of science in Egypt. In Saudi Arabia the first girls' school started in 1964 and the first college for women, which was a section of King Abdul-Aziz University (where education is not mixed), started in 1975. I was the founder of the Physics Department of this women's section. Egyptians have played significant roles in teaching schoolchildren and university students of both sexes in all the Arab countries: Saudi Arabia, Sudan, Kuwait, Yemen, the Gulf States, Libya, Lebanon, Syria, and Jordan. But with respect to Algeria, Tunisia and Morocco, our role was limited, since classes are taught in French. Arab women living in the countries located east of Egypt still have many difficulties facing them, needing to overcome many technical, academic, and social problems, while women in the countries located west of Egypt have fewer problems. There were many problems in the early days of education in Egypt but the women of Egypt worked hard to gain the same rights as men and were able to pave the way for all Arab women. I myself met many difficulties in my early days. This talk will also describe the impact of the regional conference on Women in Physics in Africa and Middle East, which was held in Cairo in 2007.

12:35PM J4.00005 Women Physicists in Asia. YOUNG-KEE KIM, Fermi National Accelerator Laboratory and University of Chicago — I will present the history of women scientists in Asian countries and discuss the current status and experiences from women physicists, and ways to create a better future for women in physics.

1:11PM J4.00006 Women in Physics: A Caribbean Perspective. KANDICE TANNER, University of California, Berkeley — This paper is concerned with aspects of post-secondary education of women in physics in the Caribbean, focusing more specifically on the main university campuses in Trinidad and Tobago, Jamaica, and Barbados. Within this framework, there are three institutions of tertiary education that provide for undergraduate and post-graduate studies in physics. On average, the bachelor-level graduating class is roughly 40% female. A great majority of these students go on to seek master's degrees in engineering. Among those enrolled in graduate programs featuring research in astronomy, materials science, environmental physics, medical physics, and quantum physics. From October 2008, 31% of all the women in physics in the 25 selected countries and from the Caribbean region are engaged in bachelor and doctoral programs in physics abroad, but no formal survey is available to provide the relevant quantitative information. However, an attempt will be made to quantify this component. Based in part on personal experience, a comparison will be made between domestic and foreign educational pathways, in terms of access to resources, level of research training, and occupational opportunities following graduation.

1:36PM J4.00007 Panel Discussion. MODERATOR: CHERRILL SPENCER, SLAC National Accelerator Laboratory — Participants: Yevgeniya Zastavker, Franklin W. Olin College of Engineering Young-Kee Kim, Fermi National Accelerator Facility and University of Chicago Karimat El-Sayed, Ain-Shams University, Cairo, Egypt Renee Horton, University of Alabama Kandice Tanner, University of California, Berkeley

Tuesday, March 17, 2009 11:15AM - 2:15PM — Session J5 DPOLY: Polymer Nanoparticle Interactions 401/402
Simulations of Polymer Grafted Nanoparticles in a Polymer Matrix

11:15AM J5.00001

SMITH, University of Utah — We have performed molecular dynamics (MD) simulations of polymer-grafted nanoparticles in a polymer melt. The model is a coarse-grained representation of spherical nanoparticles with a grafted poly(methyl methacrylate)-like bead-spring polymer in a matrix of the same polymer. Simulations were performed on both a single polymer-grafted nanoparticle as well as for a pair of polymer-grafted nanoparticles. The nanoparticle has a diameter of 5 nm. We have investigated the role of the molecular weight of the grafted and matrix polymer on both brush structure and nanoparticle-nanoparticle interactions. We find that brush density profile is independent of matrix molecular weight. Furthermore, the matrix chains penetrate almost to the particle surface, and there is no extended region with zero or near-zero matrix chain density. Hence, the highly curved brush does not exhibit “dry brush” behavior that would be expected at this investigated grafting density. We observe a repulsive interaction between the nanoparticles that sets in at a separation consistent with the polymer brush height. The combined brush-brush plus matrix effect on the nanoparticle-nanoparticle interactions is repulsive at all separations. Our simulations profile reveals no matrix-induced attraction between nanoparticles that is anticipated when the brush are truly “dry”, i.e., largely non-penetrable by the matrix. Such behavior would be expected for larger particles where the surface curvature effects on brush structure and brush-melt interactions are less important. However, for small nanoparticles, our simulations reveal that surface curvature effects are very important in determining the structure of the grafted polymer as well as nanoparticle-nanoparticle interactions.

11:51AM J5.00002

KRISHNAMOORTI, University of Houston — Grafting polymers to nanoparticles has proven to be an effective means to disperse isotropic and anisotropic nanoparticles in polymer matrices. Depending on the grafting density, polydispersity and nature of polymer - nanoparticle interaction, such grafted nanoparticles can either be liquid-like, gel-like or crystalline solids. We examine here the nature of interactions between such grafted nanoparticles and correlate those to the structure, dynamics and transport in both solvent and polymer media.

Modification of Block Copolymers Using Surface-Functionalized Hard and Soft Nanoparticles

12:27PM J5.00003

RICHARD SPONTAK, North Carolina State University — Due to their wide range of available nanostructures, ordered block copolymers provide excellent templating media into which nanoparticles can be incorporated with precise spatial modulation for various nanotechnologies. Previous experimental and theoretical studies have demonstrated that the relative size and selectivity of surface-functionalized inorganic nanoparticles can be used to tune the position of the nanoparticles along interfacial regions or within microdomains. Using a combination of experimental and theoretical methods, we furthermore show that these parameters, in addition to nanoparticle concentration, can be used to controllably alter the phase stability of block copolymers. While nanoparticles typically reduce the order-disorder transition (ODT) temperature of ordered block copolymers, a limited window exists wherein the nanoparticles increase the ODT temperature and stabilize the copolymer nanostructure. This nanoparticle-mediated design is extended in this study to include "soft" nanoparticles composed of core-shell microgels (CSMG) particles, which can be envisaged as permanent micelles. Addition of CSMG particles to ultrathin films consisting of ordered block copolymers varying in morphology and molecular weight is investigated here by electron microscopy.

Polystyrene Single Crystal Meets Nanoparticle, Toward Ordered Hybrid Materials

1:03PM J5.00004

CHRISTOPHER LI, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104 — Judiciously selected polymer single crystal (PSC) systems can interplay with 1-D and 0-D nanoparticles, forming ordered hybrid structures. In this presentation, I will first focus on patterning PSCs on individual carbon nanotubes (CNT). Using both controlled solution crystallization, thin film crystallization and physical vapor deposition methods, CNTs were periodically decorated with PSCs, resulting in nano hybrid shish-kebab (NHSK) structures. Because the polymer kebabs can be easily removed, these unique NHSKs can serve as templates to fabricate a variety of CNTs-containing hybrid materials with controlled patterning on the CNT surface. Sub-20 nanometer alternating patterning was achieved by using crystalline block copolymers. The mechanism was attributed to the crystallization induced block copolymer phase separation. This pattern was successfully used to template nanoparticles (NP) patterning on CNTs. In the second part of the talk, I will discuss fabricating Janus NPs and patterning these NPs using PSCs. Single crystals of thiol-terminated polyethylene oxide (PEO) were incubated in a gold sol. Au-S bonds were formed between the AuNPs and the PEO single crystal surfaces. The inter-particle spacing was controlled by PEO molecular weights, the incubation time, and the annealing temperatures after incubation. The planar geometry of the PSCs led to Janus NP formation. A series of NP dimers, trimers and tetramers were synthesized. NP nanowires were also fabricated. We anticipate that this observation could lead to controlled synthesis of artificial molecules and NP chains for a variety of optical, electronic, and biomedical applications.

DNA Directed Nanoparticle Assemblies

1:39PM J5.00005

FRANCIS W. STARR, Wesleyan University — While DNA is mostly noted for carrying genetic information, a single strand of DNA is simply a polymer with chemically specific recognition. As a result, DNA is an interesting polymer to consider for the development of new materials. In particular, attaching single strands of DNA to nanoparticles offers the possibility to encode highly specific binding between nanoparticles to create engineered building blocks, or “functionalized atoms.” These core units are an ideal candidate for the development of network-based, nanostructured materials. In this talk, we present results from computer simulations of a coarse-grained model examining several choices and DNA functionalization, and show how these design choices can affect dynamics, phase behavior, and the formation of crystal structures. We first discuss nanoparticles functionalized by four single DNA strands. These units give rise to a material with a hierarchy of interpenetrating networked structure and four thermodynamically distinct amorphous phases, unlike any naturally occurring pure material. On the other hand, the mechanism for the formation of the amorphous phases offers insight into anomalous networked liquids like water and silica. We also consider how varying the number of functionalizing DNA strands alters both the number and shape of these phase transitions. The formation of very low density crystals of nanoparticles tethered by DNA has recently been achieved experimentally, but the factors controlling crystal formation are still not well understood. Therefore, we also discuss the results of nanoparticles uniformly coated with DNA, similar to experimental systems. We show how the DNA strand length and stiffness affects the competition between energy and entropy that controls crystal formation.

1 Support from NSF DMR-0427239.

Tuesday, March 17, 2009 11:15AM - 2:15PM — Session J6 DCOMP: Computational Modeling of Crystallization and Nucleation Phenomena
surface induced nucleation. This is related to both the local static and dynamical properties of liquid surface.

Furthermore, in contrast to the common assumption that regards surfaces as heterogeneous center, we identify the homogeneous preferential nucleation in close proximity of free surfaces is related to the density decrease occurring upon freezing, and surface tension facilitating the initial nucleation. We provide direct computational evidence of surface induced crystallization in supercooled systems with $dP/dT < 0$. We show that the possibility of observing preferential nucleation in close proximity of free surfaces is related to the density decrease occurring upon freezing, and surface tension facilitating the initial nucleation.

The implications of coupled nucleation processes on phase formation, stability and nanoscale crystallization are discussed.

**References**


**Out-of-equilibrium processes in suspensions of oppositely charged colloids:**

**Liquid-to-crystal nucleation and gel formation.** EDUARDO SANZ

In collaboration with Chantal Valeriani, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, SUPA, School of Physics, University of Edinburgh — We study the kinetics of the liquid-to-crystal transformation and of gel formation in colloidal suspensions of oppositely charged particles. We analyse, by means of both computer simulations and experiments, the evolution of a fluid droplet quenched to a state point of the phase diagram where the most stable state is either a homogeneous crystalline solid or a solid phase in contact with a dilute gas. On the one hand, at high temperatures and high packing fractions, close to an ordered-solid/disordered-solid coexistence line, we find that the fluid-to-crystal pathway does not follow the minimum free energy route. On the other hand, a quench to a state point far from the ordered-crystal/disordered-crystal coexistence border is followed by a fluid-to-solid transition through the minimum free energy pathway. At low temperatures and packing fractions we observe that the system undergoes a gas-liquid spinodal decomposition that, at some point, arrests giving rise to a gel-like structure. Both our simulations and experiments suggest that increasing the interaction range favors crystallization over vitrification in gel-like structures.

In collaboration with Chantal Valeriani, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, Princetonplein 5, 3584 CC Utrecht, The Netherlands and SUPA, School of Physics, University of Edinburgh, JCMB King’s Buildings, Mayfield Road, Edinburgh EH9 3JZ, UK; Teun Vissers, Andrea Fortini, Mirjam E. Leunissen, and Alfons van Blaaderen, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University; Daan Frenke, FOM Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands and Department of Chemistry, University of Cambridge, Lensfield Road, CB2 1EW, Cambridge, UK; and Marjolein Dijkstra, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University.

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Institute of Science and Technology — We investigated the robustness of cellular metabolism by simulating the system-level computational models, and also performed the corresponding experiments to validate our predictions. We address the cellular robustness from the “metabolite”-framework by using the novel concept of “flux-sum,” which is the sum of all incoming or outgoing fluxes (they are the same under the pseudo-steady state assumption). By estimating the state-of-the-art high-throughput experimental techniques generate just a binary (yes or no) information about individual interactions. As a result, most of the previous research concentrated just on topology of these networks. In a series of recent publications [1-4] my collaborators and I went beyond purely topological studies and calculated the mass-action equilibrium of a genome-wide binding network using experimentally determined protein concentrations, localizations, and reliable binding interactions in baker’s yeast. We then studied how this equilibrium responds to large perturbations [1-2] and noise [3] in concentrations of proteins. We demonstrated that the change in the equilibrium concentration of a protein exponentially decays (and sign-alternates) with its network distance away from the perturbed node. This explains why, despite a globally connected topology, individual functional modules in such networks are able to operate fairly independently. In a separate study [4] we quantified the interplay between specific and non-specific binding interactions under crowded conditions inside living cells. We show how the need to limit the waste of resources constrains the number of types and concentrations of proteins that are present at the same time and at the same place in yeast cells.


Financial support by EU-STREP NANOPHOTO project and by “Fondazione Banco di Sardegna” is acknowledged.

Tuesday, March 17, 2009 11:15AM - 2:15PM – Session J7 GSNP DBP: Complex Cellular Biological Networks 407

11:15AM J7.00001 Mass-action equilibrium and non-specific interactions in protein binding networks1, SERGEI MASLOV, Brookhaven National Laboratory — Large-scale protein binding networks serve as a paradigm of complex properties of living cells. These networks are naturally weighted with edges characterized by binding strength and protein-nodes – by their concentrations. However, the state-of-the-art high-throughput experimental techniques generate just a binary (yes or no) information about individual interactions. As a result, most of the previous research concentrated just on topology of these networks. In a series of recent publications [1-4] my collaborators and I went beyond purely topological studies and calculated the mass-action equilibrium of a genome-wide binding network using experimentally determined protein concentrations, localizations, and reliable binding interactions in baker’s yeast. We then studied how this equilibrium responds to large perturbations [1-2] and noise [3] in concentrations of proteins. We demonstrated that the change in the equilibrium concentration of a protein exponentially decays (and sign-alternates) with its network distance away from the perturbed node. This explains why, despite a globally connected topology, individual functional modules in such networks are able to operate fairly independently. In a separate study [4] we quantified the interplay between specific and non-specific binding interactions under crowded conditions inside living cells. We show how the need to limit the waste of resources constrains the number of types and concentrations of proteins that are present at the same time and at the same place in yeast cells.


1. Work at BNL was carried out under Contract No. DE-AC02-98CH10886, Division of Material Science, U.S. Department of Energy.

12:27PM J7.00003 Synthetic rescues and spontaneous cascades in metabolic networks1, ADILSON E. MOTTER, Northwestern University — Using in silico experiments, I will show that organisms evolving to maximize growth rate, ATP production, or any other linear function of metabolic fluxes tend to significantly reduce the number of active metabolic reactions compared to typical non-optimal states. The reduced number appears to be constant across the microbial species studied and just slightly larger than the minimum number required for the organisms to grow at all. I will show that this massive reaction silencing is triggered by the irreversibility of a large fraction of the metabolic reactions and propagates through the network as a cascade of inactivity. Following these significant observations, I will introduce a network method to recover the loss of metabolic function due to mutations and other defects, which is based on bypassing rather than correcting the defective pathways. In particular, I will present predictions of synthetic recovery, in which the knock-out of one enzyme-coding gene results in a non-viable phenotype while the concurrent knock-out of a second enzyme-coding gene restores viability. In addition to their potential role in metabolic engineering and medical research, these results have puzzling implications for the recently observed temporary activation of latent pathways.


1:03PM J7.00004 Robustness of metabolic networks, HAWOONG JEONG, Department of Physics, Korea Advanced Institute of Science and Technology — We investigated the robustness of cellular metabolism by simulating the system-level computational models, and also performed the corresponding experiments to validate our predictions. We address the cellular robustness from the “metabolite”-framework by using the novel concept of “flux-sum,” which is the sum of all incoming or outgoing fluxes (they are the same under the pseudo-steady state assumption). By estimating the changes of the flux-sum under various genetic and environmental perturbations, we were able to clearly decipher the metabolic robustness; the flux-sum around a metabolite does not change much under various perturbations. We also identified the list of the metabolites essential to cell survival, and then “acclimator” metabolites that can control the cell growth were discovered. Furthermore, this concept of “metabolite essentiality” should be useful in developing new metabolic strategies to improve the production of various bioproducts and designing new drugs that can fight against multi-antibiotic resistant superbacteria by knocking-down the enzyme activities around an essential metabolite. Finally, we combined a regulatory network with the metabolic network to investigate its effect on dynamic properties of cellular metabolism.
1:39PM J7.00005 Discrete dynamic modeling of T cell survival signaling networks, RANRAN ZHANG, Pennsylvania State University — Biochemistry-based frameworks are often not applicable for the modeling of heterogeneous regulatory systems that are sparsely documented in terms of quantitative information. As an alternative, qualitative models assuming a small set of discrete states are gaining acceptance. This talk will present a discrete dynamic model of the signaling network responsible for the survival and long-term competence of cytotoxic T cells in the blood cancer T-LGL leukemia. We integrated the signaling pathways involved in normal T cell activation and the known deregulations of survival signaling in leukemic T-LGL, and formulated the regulation of each network element as a Boolean (logic) rule. Our model suggests that the persistence of two signals is sufficient to reproduce all known deregulations in leukemic T-LGL. It also indicates the nodes whose inactivity is necessary and sufficient for the reversal of the T-LGL state. We have experimentally validated several model predictions, including: (i) Inhibiting PDGF signaling induces apoptosis in leukemic T-LGL. (ii) Sphingosine kinase 1 and NFκB are essential for the long-term survival of T cells in T-LGL leukemia. (iii) T box expressed in T cells (T-bet) is constitutively activated in the T-LGL state. The model has identified potential therapeutic targets for T-LGL leukemia and can be used for generating long-term competent CTL necessary for tumor and cancer vaccine development. The success of this model, and of other discrete dynamic models, suggests that the organization of signaling networks has an determining role in their dynamics. Reference: R. Zhang, M. V. Shah, J. Yang, S. B. Nyland, X. Liu, J. K. Yun, R. Albert, T. P. Loughran, Jr., Network Model of Survival Signaling in LGL Leukemia, PNAS 105, 16308-16313 (2008).

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J8 FEId FIAP: Preparing Physics Students for Careers in Industry 414/415

11:15AM J8.00001 The Physics Workforce: The Latest Data on Supply and Demand, ROMAN CZUJKO, American Institute of Physics — This paper will provide an overview of the trends both in physics education at all degree levels and in the employment of physicists throughout the economy. The paper also includes comparative data on the trends in related fields. There will be a discussion of the common career paths pursued by physicists at different degree levels with particular emphasis on non-academic employment. The paper includes a detailed description of professional master’s degree programs in physics departments as well as findings from AIP* studies that describe the skills that employers value. The paper concludes with suggestions for how physics departments might assist their students in finding employment during these difficult economic times.

11:51AM J8.00002 Industrial Physics Careers: A Large Company Perspective, STEFAN ZOLLNER, IBM — Statistical data from the American Institute of Physics and the National Science Foundation show that only about a third of physics graduates get permanent jobs in academia. A few work in government labs and hospitals. The majority of physics Ph.D.s, however, find employment in the private sector (industry). This trend has been increasing, i.e., recent Ph.D.s are even more likely to start careers in industry. Industrial physicists work in small, medium or large companies in a broad range of fields, including aerospace, semiconductors, automotive, energy, information technology, contract research, medical, chemical, optics, etc. They are also represented in fields outside of physics, such as finance. Even the “inventor” of the Powerball lottery game is a Ph.D. physicist. In my talk, I will describe pathways to success for an industrial physicist, from the perspective of employment in three different large corporations. Based on the NIST Baldridge criteria of Performance Excellence, I will discuss how to achieve and measure organizational success through focus on products and customers. Individual performance is linked to the goals of the organization. Performance has two components: Goals and behaviors. Both are key to success as an individual contributor or manager.

References:
http://www.aps.org/about/governance/committees/commemb/index.cfm
http://www.quality.nist.gov/

12:27PM J8.00003 The Rutgers Undergraduate Physics Program: Preparing Students for Varied Careers, MOHAN KALELKAR, Rutgers University — At Rutgers University we offer three main physics major tracks, each tailored towards different kinds of career aspirations. The Professional Option is for students who intend to go on to physics graduate study. The Applied Option is for students who desire technical jobs in industry, but without graduate study. The General Option is for students who have an interest in physics, but do not aspire to a technical career. I will discuss how these Options prepare students for their desired careers, and will give specific examples of jobs obtained. I will especially focus on the Applied Option, explaining how it has evolved based on lessons learned, and what further steps we need to take at Rutgers. I will close by briefly discussing a new, fourth physics major track we have just introduced, our Ocean Physics Option. I will describe this new Option and discuss prospects for its success.

1:03PM J8.00004 ABSTRACT WITHDRAWN –

1:39PM J8.00005 Training PhD Physicists for Industrial Careers: The Industrial Leadership in Physics Program at Georgetown University, EDWARD VAN KEUREN, Department of Physics, Georgetown University — The Physics department at Georgetown University has a unique PhD level graduate program designed to prepare PhD physicists for positions in high-tech business. Launched in 2001, the Industrial Leadership in Physics (ILP) graduate program combines training in technical subjects and business topics with a focus on group learning, communication skills, and practical work experience. Some highlights of the program include a modular curriculum in fundamental physics, centered on solid-state physics, instrumentation, problem solving and computer modeling; a year-long apprenticeship at the site of an industrial partner chosen to match the interests of the student and coursework in the McDonough School of Business at Georgetown. This presentation will give an overview of the program.

Tuesday, March 17, 2009 11:15AM - 2:03PM –
Session J9 GSNP: Focus Session: Elasticity and Geometry of Thin Objects II 303

11:15AM J9.00001 The self assembly of closed surfaces from flat sheet, MICHAEL BRENNER, Applied Mathematics and Applied Physics, School of Engineering and Applied Sciences, Harvard University — We will discuss theoretical and some experimental work to understand the conditions which a flat sheet with embedded permanent magnets can spontaneously fold into a closed surface. The critical question is understanding how to design the system — both the cut of the sheet and the position of the magnets — to maximize the yield of assembling into a closed surface without misfolding. This problem also raises novel and interesting questions in thin plate elasticity, which will be highlighted.
phenomena such as spontaneous buckling and the emergence of a boundary layer. When the prescribed reference curvatures and 2D metric do not comply with one another, the system is frustrated (non-Euclidean). Such systems exhibit various behaviors: sheets with imposed positive Gaussian curvature have weak thickness dependence, their bending content is bounded and their total bending energy scales like thickness cube. On the other hand, sheets with imposed negative Gaussian curvature undergo a set of bifurcations, as they obtain configurations uniformly when heated above 33°C. This process prescribes a non-Euclidean “target” metric on the sheets. In order to reduce their energy, the plates buckle with a wavelength proportional to the interaction range. This model can be simulated on a random mesh, which can be defined on any arbitrary curved geometry. Through these simulations, we determine how stripped phases respond to curvature on spheres, tori, and other geometries.

12:03PM J9.00003 Simulating Complex Modulated Phases Through Spin Models, JONATHAN V. SELINGER, LENA M. LOPATINA, JUN GENG, ROBİN L. B. SELINGER, Kent State University — We extend the computational approach for studying stripped phases on curved surfaces, presented in the previous talk, to two new problems involving complex modulated phases. First, we simulate a smeared liquid crystal on an arbitrary mesh by mapping the director field onto a vector spin and the density wave onto an Ising spin. We can thereby determine how the smectic phase responds to any geometrical constraints, including hybrid boundary conditions, patterned substrates, and disordered substrates. This method may provide a useful tool for designing ferroelectric liquid crystal cells. Second, we explore a model of vector spins on a flat two-dimensional (2D) lattice with long-range antiferromagnetic interactions. This model generates modulated phases with surprisingly complex structures, including 1D stripes and 2D periodic cells, which are independent of the underlying lattice. We speculate on the physical significance of these structures.
When the self-interaction of the SQD becomes significant. We explore these three regimes in detail and set bounds on each.

As the coupling is further increased by increasing the sizes of both the SQD and the MNP, we find a regime of bistability. This originates by increasing the size of the SQD, we find a double peaked Fano structure in the response. This second peak occurs when the induced field becomes stronger field limit that each exhibit novel properties. In the first regime, we find that the energy absorption spectrum displays an asymmetrical Fano shape (as previously

Bryant, NIST, Gaithersburg — We study the optical response of a semiconductor quantum dot (SQD) coupled with a metal nanoparticle (MNP). In particular,

we explore the relationship between the size of the constituents and the response of the system. We identify, three distinct regimes of behavior in the strong

Bryant, NIST, Gaithersburg — We study the optical response of a semiconductor quantum dot (SQD) coupled with a metal nanoparticle (MNP). In particular,

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1:27PM J9.00010 Wrinkles/Folds and the Role of Interfacial Thermodynamics 1, LUKA POČIVAVŠEK, BRIAN LEAHY, The University of Chicago, ENRIQUE CERDA, Universidad de Santiago de Chile, BINUHA LIN, KA YEE LEE, The University of Chicago — We recently developed a general model for studying instabilities like wrinkling and folding in interfacial membranes on fluid substrates. The dominant length scales describing the instability are set by the elastic response of the membrane (primarily bending) and the “stiffness” of the substrate. These length scales, like the wrinkle wavelength and fold amplitude, are independent of the particular interfacial molecular interactions for micron thick membranes where typical system energies like the membrane bending stiffness are thousands of times larger than intermolecular potentials. However, as the membranes become thinner and the chemical interactions between the membrane and the fluid substrate strongly influence the wrinkling and folding length scales. We present data for two such systems (a lipid monolayer and a gold nanoparticle layer) on different hydrogen bonding fluids and discuss possible mechanisms and modifications of our wrinkle-to-fold scaling laws to account for this new degree of freedom.

1:39PM J9.00011 Universal Shapes of Interacting Mode-I Cracks, MELISSA FENDER, FREDERIC LECHEAULT, Dept. of Physics, North Carolina State University, PEDRO REIS, Dept. of Mathematics, MIT, BENÖIT ROMAN, P.M.M.H, UMR 7636 CNRS/ESPCI/Paris6,Paris7, KAREN DANIELS, Dept. of Physics, North Carolina State University — We experimentally investigate the interaction between two parallel cracks propagating towards each other under uniaxial traction in quasi-2D slabs of gelatin. A single crack would propagate perpendicular to the direction of traction. However, after they pass each other, the two cracks rotate and ultimately meet, leaving behind a lens-shaped remnant. We find a universal length-to-width ratio for this remnant, independent of the pulling speed and initial crack separation; the same phenomenon is observed in a variety of elastic materials. Moreover, the overall dimensions of the lens-shaped remnant are set by the initial crack separation.

1:51PM J9.00012 The Life and Times of a Ruck in a Rug, DOMINIC VELLA2, MOHTKAR ADDA-BEDIA, AREZKI BOUDAOU, LPS ENS, Paris — We study the familiar problem of a ruck in a rug. Under lateral compression, a rug bends out of the plane forming a ruck — a localised region in which it is no longer in contact with the floor. We consider the equilibrium of such a ruck. Once the external force that caused the compression is removed, experience tells us that the ruck may either remain or flatten out under its own weight. We quantify the conditions under which each of these two scenarios occurs. We also consider how the propagation of a ruck along the carpet facilitates large-scale sliding.

1 Also: DAMTP, Cambridge

Tuesday, March 17 2009 11:15AM - 2:15PM —
Session J10 DMP: Focus Session: Optical Properties of Nanostructures II: Quantum-Dot-Coupled Systems 304

11:15AM J10.00001 Optical Detection and Control of Single Magnetic Ions in Photonic Microcavities1, 2, DAVID D. AWSCHALOM2, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — As the density of magnetic information storage scales upwards, their spin lifetimes increase with decreasing concentration as the ions become isolated. Here we describe the spatially-resolved observation and manipulation of isolated Mn spins integrated within photonic microcavities. A single magnetically-doped GaAs quantum well is fabricated within both microdisk and vertical Fabry-Perot cavities in which their respective cavity modes are coupled to the neutral Mn acceptor emission. Scanning micro-photoluminescence measurements reveal cavity-coupled emission and a dramatic increase in the measured signal to noise ratio, thereby allowing direct imaging of narrow linewidth luminescence from the Mn moments. These Mn ion spins are optically polarized at zero-field, exhibit long spin lifetimes, and may be manipulated through a variety of techniques.

1This work was supported by the NSF and the ONR.

2In collaboration with R. C. Myers, G. Calusine, T.-L. Liu, and E. Hu.


11:51AM J10.00002 ABSTRACT WITHDRAWN —

12:03PM J10.00003 Silicon nanocrystal photoluminescence in cylindrical whispering gallery resonators, P. BIANUCI, Department of Physics, University of Alberta, Edmonton AB, T6G 2G7, Canada, J.R. RODRIGUEZ, Department of Chemistry, University of Alberta, Edmonton AB, T6G 2G2, Canada, C.M. CLEMENTS, Department of Physics, University of Alberta, Edmonton AB, T6G 2G7, Canada, J.G.C. VEINOT, Department of Chemistry, University of Alberta, Edmonton AB, T6G 2G2, Canada, A. MELDRUM, Department of Physics, University of Alberta, Edmonton AB, T6G 2G7, Canada — We present photoluminescence studies of Silicon-nanocrystal (Si-NC) coated cylindrical microcavities. The coatings were prepared by dip-coating standard optical fibers with a solution-based precursor followed by a high-temperature annealing step. The photoluminescence spectra measured perpendicular to the fiber axis show high Q-factor (~2500) whispering gallery modes, and allows distinction between TE and TM modes. We also show a proof-of-principle implementation of a far-field refractometric sensor using a nanocrystal-coated fiber.

12:15PM J10.00004 Optical Response of Strongly Coupled Quantum Dot-Metal Nanoparticle Systems: Double Peaked Fano Structure and Bistability, RYAN ARTUSO, University of Maryland College Park, GARNETT BRYANT, NIST, Gaithersburg — We study the optical response of a semiconductor quantum dot (SQD) coupled with a metal nanoparticle (MNP). In particular, we explore the relationship between the size of the constituents and the response of the system. We identify, three distinct regimes of behavior in the strong field limit that each exhibit novel properties. In the first regime, we find that the energy absorption spectrum displays an asymmetrical Fano shape (as previously predicted). It occurs when there is interference between the applied field and the induced field produced by the SQD at the MNP. When the coupling is increased by increasing the size of the SQD, we find a double peaked Fano structure in the response. This second peak occurs when the induced field becomes stronger than the external field. The coupling is further increased by increasing the sizes of both the SQD and the MNP, we find a regime of bistability. This originates when the self-interaction of the SQD becomes significant. We explore these three regimes in detail and set bounds on each.
12:27PM J10.00005  Excitons and plasmons in coupled nanoparticles and nanowires. PEDRO L. HERNANDEZ-MARTINEZ, ALEXANDER O. GOVOROV, Ohio University — In this study, we develop theoretical models of coupled nanoparticles (NPs) and nanowires (NWs). In particular, we focus on exciton energy transfer between NPs and NWs and consider both metal and semiconductor nanocrystals. We obtain analytical equations for the long distance limit and a numerical solution for the general case. For long distances, the energy transfer rate is proportional to 1/d^5, where d is the distance between NP and NW [1]. In a coupled NP-NW structure, excitonic energy can be efficiently extracted and channelled to nanowires/nanotubes by utilizing the Förster energy transfer mechanism [1,2]. The calculated energy transfer rates are in good agreement to the experimental values [2]. The NP-NW system has potential for applications in optoelectronic devices and sensors [3]. [1] P. Hernandez-Martinez, A. O.Govorov, Phys. Rev. B 78, 035314 (2008). [2] J. Lee, A. O. Govorov, and N. A. Kotov, Nano Letters 5, 2063-2069 (2005). [3] J. Lee, P. Hernandez, J. Lee, A. O. Govorov, and N. A. Kotov, Nature Materials, 6, 291 – 295 (2007).

12:39PM J10.00006  High-transmission ridge nanoapertures for quantum dot devices1. AKIHIRO KIRIHARA, JUNICHI FUJIKATA, NEC Corporation, TOSHIHIRO NAKAOKA, NAOTO KUMAGAI, KATSUYUKI WATANABE, University of Tokyo, MASAYUKI SHIRANE, SHUNSUKI OHKOUCHI, SHINICHI YOROZU, NEC Corporation, YASUHIKO ARAKAWA, University of Tokyo — We report on double-ridge apertures to enhance the coupling between a single quantum dot (QD) and optical field. The double-ridge aperture has two metallic tips protruding inward and facing each other, which work as an effective antenna for a QD just below the tips. We performed FDTD simulation to optimize the apertures, and fabricated them on InAs/GaAs QDs emitting at 960nm. By single-dot PL spectroscopy through the double-ridge aperture, we demonstrated 5-6 times enhancement in PL extraction efficiency, compared to that through a conventional circular aperture. Because our double-ridge aperture works not only as an optical antenna but also as an electrode for a QD, it will be applicable to electrically-driven photon generators or photon detectors.

1This work was supported by Japanese Special Coordination Funds for Promoting Science and Technology.

12:51PM J10.00007  Polarization and Angle Dependent Spontaneous Emission Rates in Hybrid Metal-Semiconductor Nanostructures, YIKUAN WANG, TIANYU YANG, MARK TUOMINEN, MARC ACHERMANN, University of Massachusetts Amherst — Recently, the coupling of a dipole emitter to surface plasmons (SPs) of metal nanostructures has attracted much attention for its potential applications in light emitting devices. Our time-resolved photoluminescence (PL) study on the emission of CdSe/ZnS core/shell nanocrystals (NCs) deposited on a two-dimensional array of gold nanodiscs demonstrates that the spontaneous emission of dipole emitters is strongly dependent on the detection angles and polarizations. The in-plane, s-polarized PL measurements are independent on detection angles, and can be described by the PL decay dynamics of two NC subsets: the emission from NCs on the dielectric substrate and from NCs on the gold nanodiscs that experience non-radiative quenching by the metal.

The out-of-plane, p-polarized PL measurements show an additional decay caused by SP-induced enhancement of the spontaneous emission rate. This angular-dependent enhancement is explained by interactions between NC dipole moments and the out-of-plane SP resonance of the gold nanodiscs.

1:03PM J10.00008  Decay-rate distribution of single quantum dots in nanometer-scale proximity to a metal film. MATTHEW PELTON, XIAOHUA WU, Argonne National Laboratory — Recently, the interaction between fluorescent colloidal semiconductor quantum dots and plasmonic metal nanostructures has attracted great interest, both for the development of a basic understanding of nanoscale photophysics and for potential applications in improved light-emitting devices and integrated plasmonic circuits. Time-resolved measurements on single dots are required in order to overcome the obscuring effects of ensemble averaging and of time averaging, and thus reveal the physical mechanisms of dot-metal interaction. In this work, we present measurements of photoluminescence decay dynamics from single colloidal CdSe/ZnS core-shell quantum dots in nanometer-scale proximity to a smooth gold film. We extract the decay rate, k_ν, for each dot when it is in its maximum-intensity state, thereby removing the effects of nonradiative decay-rate fluctuations. We find that, as the separation between the dot and the metal decreases, the k_ν distribution becomes broader and its maximum increases. The increase in maximum decay rate is caused by stronger energy transfer from the quantum dot to the metal film, as expected. The broader distribution of decay rate, on the other hand, reflects inherent variations in the interactions between individual dots and the metal film.

1:15PM J10.00009  Demonstration of Optical Resonances in a Cylinder-Shell Lattice of Quantum Dots, JARED MAXSON, SLAVA ROTKIN, Department of Physics, Lehigh University — We present a model for the calculation of the optical response of a cylinder-shell quantum dot or metallic nanostructures. Our model is a shell cluster as a lattice of non-permanent point dipoles with a known polarization and a single transition frequency. We then utilize the second quantization formalism to compute the cluster response. The eigenmodes and quantum mechanical response function of the lattice interacting with an external field, polarized respective to the cylinder axis, are calculated numerically. The cylinder radius is treated as a parameter to identify resonator metallic effects due to the cylindrical geometry. Varying the frequency of the external field, regions of response maxima are determined. In these regions resonant interaction between the coupled dipoles results in transferring significant oscillator strength into a few eigenmodes of the cluster, having high spatial and temporal coherence with the external field. Further analysis of the spatial distribution of eigenstates in each region of response maxima reveals significant contributions from groups of modes with equal angular momenta, permitting rigorous excitation classification.

1:27PM J10.00010  Two-Photon Transitions in Molecular Quantum Dot System, MICHAEL SCHEIBNER, ILYA PONOMAREV, DANNY KIM, ALLAN BRACKER, DANIEL GAMMON, Naval Research Laboratory — Two-photon excitations are at the heart of important nonlinear optical processes and provide a key to the rich physics and fresh opportunities of designer quantum materials. In this study we consider double dot quantum dot molecules (QDMs) that were designed by molecular beam epitaxial growth to exhibit either electron or hole tunnel coupling of the two dots. The electron or hole levels of the two dots can be tuned into resonance with applied electric field created by Schottky diode structure. We demonstrate that, by using two polarizations of two photon transitions, one can control the absorption spectrum of the molecular biexciton in such a QDM. We identify a new two-photon transition which is the first example of a simultaneous, coherent optical excitation of a pair of QDs in a weakly coupled regime. We further show that a photoluminescence excitation measurement with stereo-chromatic detection can be used to gain access to the spin physics in this regime.

1:39PM J10.00011  Qubit extraction and manipulation in optically-driven self-assembled quantum dot molecules.1, J.E. ROLON, S.E. ULOA, Ohio University — Semiconductor quantum dot molecules (QDMs) allow studies of different mechanisms of coherent optoelectronic control of excitative states in the pursuit of stable and well characterized qubits. In this work, we develop a realistic calculation of the dressed spectrum and exciton dynamics of InAs/GaAs QDMs. The dressed spectrum contains electron and hole tunneling as well as exciton Förster resonant energy transfer (FRET) level anticrossing signatures, from which we derive an effective Hamiltonian using a projection operator formalism. The state dynamics is analyzed using a multilevel Lindblad master equation, in which the projected density matrix is obtained by partial tracing of the irrelevant exciton degrees of freedom. We find that the interplay of FRET and carrier tunneling can produce a charge qubit subspace whose indirect exciton character makes it resilient to lifetime limited decoherence. Furthermore, it is shown that a set of universal quantum gates can be constructed and its unitarity assured by the application of an external electric field that prevents the mixture of qubit subspace dynamics with other excitonic degrees of freedom, present upon optical excitation.

1Supported by NSF-DMR MWN and OU-BNNT.
and bias. Properties of open quantum dots, in which QPC conductances are quantized.

We have investigated the transport properties of a 1.5 µm lateral GaAs/AlGaAs quantum dot molecules under lateral electric field using empirical pseudopotentials and configuration interaction. Our model structure is directly taken from recent experiments where an In-poor basin develops below the dot. The coupling of the electron states is significantly enhanced by the presence of the basin, while the holes remain mainly uncoupled. At the proper electric field —between 0 V/cm and 200 V/cm, depending on the dot molecule—the electron states can be tuned to be evenly distributed between both dots, forming bonding and antibonding states. The optical absorption is shown to exhibit two bright transitions, mostly independent of the applied field. In emission, we argue that a fast electron-dynamics must be introduced, since the electrons are not subject to a true potential barrier between the dots and consequently only the lowest of the electron states is occupied. Following this approach, we obtain only one bright peak at high electric fields and two peaks (at higher temperature, four peaks) at the tuning point of the electron states. The results are shown to compare very well with recent experiments. A simple 4x4 Hamiltonian is derived to explain the results in the intuitive dot-localized basis.

Tuesday, March 17, 2009 11:15AM - 2:15PM  Session J11 DCMP: Quantum Dots and Quantum Point Contacts  305

11:15AM J11.00001 Imaging a One Dimensional Quantum Dot in an InAs/InP Nanowire 1. ERIN E. BOYD, HALVAR J. TRODAHL,ERIN E. BOYD, HALVAR J. TRODAHL, Max Planck Institute for Solid State Research — We calculate the electronic and optical properties of laterally coupled InGaAs quantum dot molecules under lateral electric field using empirical pseudopotentials and configuration interaction. Our model structure is directly taken from recent experiments where an In-poor basin develops below the dot. The coupling of the electron states is significantly enhanced by the presence of the basin, while the holes remain mainly uncoupled. At the proper electric field —between 0 V/cm and 200 V/cm, depending on the dot molecule—the electron states can be tuned to be evenly distributed between both dots, forming bonding and antibonding states. The optical absorption is shown to exhibit two bright transitions, mostly independent of the applied field. In emission, we argue that a fast electron-dynamics must be introduced, since the electrons are not subject to a true potential barrier between the dots and consequently only the lowest of the electron states is occupied. Following this approach, we obtain only one bright peak at high electric fields and two peaks (at higher temperature, four peaks) at the tuning point of the electron states. The results are shown to compare very well with recent experiments. A simple 4x4 Hamiltonian is derived to explain the results in the intuitive dot-localized basis.

1 Supported by the NSF grant PHY-06-46094.

11:27AM J11.00002 Imaging Double Quantum Dots in InAs/nP Nanowires. HALVAR J. TRODAHL, ERIN E. BOYD, R. M. WESTERVELT, Dept. of Physics and Sch of Eng and App Sci, Harvard Univ, LINUS E. FROBERG, KRISTIN NILSSON, LARS SAMUELSON, Dept of Solid State Physics, Lund Univ — Coupled quantum dots formed in InAs/nP heterostructure nanowires are attractive candidates for non-electronic, spintronic and quantum information processing. The ability to manipulate the charge state of a single quantum dot defined in these nanowire systems using a low temperature scanning probe microscope (SPM) tip has been shown previously [1] and provides a tool to investigate the properties of nanowire systems down to the tens of nanometer scale. In order to realize the above applications, multiple InAs quantum dots can be formed in an InAs/nP nanowire system by using InP barriers. Using a conducting SPM tip as a movable electrostatic gate, the charge can be tuned independently on each dot of a double quantum dot defined in a semiconductor nanowire. [1] A. C. Bleszynski-Jayich, et al. Synchrotron Radiation News 21, 153 (2008)

11:39AM J11.00003 Phase Coherence and Mesoscopic Coulomb Blockade in Open Quantum Dots. ILEANA RAU, MICHAEL GROBIS, SAMI AMASHA, RON POTOK, Stanford University, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDBABER-GORDON, Stanford University — The phase coherence of electrons in open systems at low temperatures leads to mesoscopic effects such as universal conductance fluctuations and weak localization of electrons. These effects are encountered in open large quantum dots and are explained by a model of non-interacting electrons. We have investigated the transport properties of a 1.5 µm<sup>2</sup> and a 3 µm<sup>2</sup> lateral GaAs/AlGaAs quantum dot in the open regime. The weak localization effect is complicated at low temperatures by the presence of residual interactions (Mesoscopic Coulomb Blockade) that persists even when the dot is coupled by one or two fully transmitting modes to each of the two leads. We present measurements of the electron dephasing rate at low temperatures in the open quantum dots and discuss how they are affected by the suppression of conductance by these Coulomb blockade effects.

11:51AM J11.00004 Mesoscopic Coulomb Blockade in a Quantum Dot with Two Open QPCs. SAMI AMASHA, ILEANA RAU, MICHAEL GROBIS, RON POTOK, Stanford University, HADAS SHTRIKMAN, Weizmann Institute, DAVID GOLDBABER-GORDON, Stanford University — A quantum dot consists of a confined droplet of electrons connected to an electron reservoir by two quantum point contacts (QPCs). When the conductance of each of these QPCs is less than 2e<sup>2</sup>/h, the dot is in the closed regime and Coulomb Blockade effects dominate the transport properties. Open quantum dots, in which QPC conductances are 2e<sup>2</sup>/h or above, are generally thought to be well-described by non-interacting electron theory. While Mesoscopic Coulomb Blockade (MCB) effects can occur in a quantum dot with one open and one closed QPC, these effects are expected to be absent for quantum dots with two open QPCs. We have investigated the transport properties of a 1.5 µm<sup>2</sup> and a 3µm<sup>2</sup> lateral GaAs/AlGaAs quantum dot in the open regime and find a clear signature of MCB. We will discuss the dependence of MCB on various controllable parameters, including magnetic field, temperature, and bias.

This work was supported by ARO.
12:03PM J11.00005 Quantum Phase Transition to a Zigzag Wigner Crystal 1 \textsuperscript{,} A. C. MEHTA, Duke University, C. J. UMRIGAR, Cornell University, A. D. GUCLU, National Research Council of Canada, K. A. MATVEEV, Argonne National Lab, H. U. BARANGER, Duke University — We use Quantum Monte Carlo techniques to map out the phase diagram of interacting electrons in a quantum wire. Interacting quasi-one-dimensional systems provide excellent examples of quantum phase transitions that are tractable. Previous work gave a qualitative description of the phase diagram of a quasi-one-dimensional system [Meyer, Matveev, and Larkin, PRL 2007]. At low density, electrons confined to one dimension by a transverse harmonic potential form a linear one dimensional Wigner crystal; as the density increases, symmetry about the axis of the wire is broken and there is a transition to a quasi-one-dimensional zigzag crystal. We use variational and diffusion Monte Carlo to study the phase diagram of this system quantitatively.

1Supported in part by the NSF (DMR-0506953).

12:15PM J11.00006 Quantum Phase Transition in a single-molecule Quantum Dot, N. ROCH, S. FLORENS, V. BOUCHIAT, W. WERNSDORFER, F. BALESTRO, Nöel Institut, Grenoble, France, NANOSCIENCES DEPARTMENT COLLABORATION — Quantum criticality is the intriguing possibility offered by the laws of quantum mechanics when the wave function of a many-particle physical system is forced to evolve continuously between two distinct, competing ground states. This phenomenon, often related to a zero-temperature magnetic phase transition, can be observed in several strongly correlated materials such as heavy fermion compounds or possibly high-temperature superconductors, and is believed to govern many of their fascinating, yet still unexplained properties. In contrast to these bulk materials with very complex electronic structure, artificial nanoscale devices could offer a new and simpler vista to the comprehension of quantum phase transitions. This long-sought possibility is demonstrated by our work in a fullerene molecular junction, where gate voltage induces a crossing of singlet and triplet spin states at zero magnetic field. N. Roch, S. Florens, V. Bouchiat, W. Wernsdorfer & F. Balestro, Quantum phase transition in a single-molecule quantum dot, Nature, 2008, 453, 633-637.

12:27PM J11.00007 Aharonov-Bohm-type interference effects in narrow gap semiconductor heterostructures, R.B. LILLIANFELD, R.L. KALLAHER, J.J. HEREMANS, Virginia Tech, HONG CHEN, University of North Florida, N. GOEL, S.J. CHUNG, M.B. SANTOS, University of Oklahoma, W. VAN ROY, G. BORGHS, IMEC (Belgium) — We present experiments on quantum interference phenomena in semiconductors with strong spin-orbit interaction, using mesoscopic parallel ring arrays fabricated on InSb/InAsSb and InAs/AlGaSb heterostructures. Both external electric field effects and temperature dependence of the ring magnetoresistance are examined. Top-gate voltage-dependent oscillations in ring resistance in the absence of an external magnetic field are suggestive of Aharonov-Casher interference. At low magnetic fields the ring magnetoresistance is dominated by oscillations with $h/2e$ periodicity characteristic of Altschuler-Aronov-Spivak (AAS) oscillations, whereas the $h/e$ periodicity characteristic of Aharonov-Bohm (AB) oscillations persists to high magnetic fields. Fourier spectra (FS) reveal AB amplitudes on the same order as AAS amplitudes at low fields, and in some samples reveals a splitting of the AB peaks, which has been interpreted as a signature of Berry’s phase. The FS are also used to quantify the temperature dependence of the oscillation amplitudes (NSF DMR-0618235, DOE DE-FG02-08ER4652, NSF DMR-0920550).

12:39PM J11.00008 Time-resolved detection of single-electron interference, SIMON GUSTAVSSON, Massachusetts Institute of Technology, MATTHIAS STUDER, ETH Zurich, RENAUD LEURTQURC, IEMN-CNRS, France, THOMAS IHN, KLAUS ENSSLIN, ETH Zurich, D. C. DRISCOLL, A. C. GOSSARD, University of California, Santa Barbara — We demonstrate real-time detection of single electron interference in a double quantum dot embedded in an Aharonov-Bohmer interferometer, with visibility approaching unity [1]. We use a quantum point contact as a charge detector to perform time-resolved measurements of single-electron tunneling. With increased bias voltage across the quantum point contact a back-action is exerted on the interferometer leading to decoherence. We attribute this to emission of radiation from the quantum point contact, which drives electronic transitions in the quantum dot [2]. Surprisingly, the efficiency of this process depends strongly on external magnetic field, with variations occurring on a small fraction of the magnetic field scale associated with one flux quantum penetrating the ring. The unexpected features demonstrate the complex interplay between radiation, absorption and coherence in mesoscopic systems. [1] S. Gustavsson et al., Nano Lett. 8, 2547 (2008). [2] S. Gustavsson et al., PRL 99, 206804 (2007).

12:51PM J11.00009 Non-equilibrium Charge Fluctuations as a Source of Inelastic Back-action in Quantum Point Contact Qubit Detectors, CAROLYN YOUNG, AASHISH CLERK, McGill University — Many recent experiments make use of a quantum point contact (QPC) as a qubit readout (e.g., of a double quantum dot (DQD) qubit). It has long been realized that QPC current fluctuations can give rise to inelastic back-action effects on the DQD [1] [2]. In contrast, the role of QPC charge fluctuations in generating inelastic back-action has not been fully studied, despite the fact that this is a more fundamental mechanism. We provide a full theoretical study of charge-noise induced inelastic back-action effects in a QPC plus DQD system, showing that these effects should be appreciable in typical experimental setups. We also discuss a novel contribution to the charge noise associated with the physics of Friedel oscillations. Finally, we discuss how the effects of charge noise back-action can be distinguished from current noise back-action in experiment.


1:03PM J11.00010 Hole Spin Filtering by quantum point contacts, TAISUKE MINAGAWA, YULI LYANDER-GELLER, Department of Physics, Purdue University — We calculate the charge carrier spectra in two-dimensional hole systems (2DHS) and in quantum point contacts (QPC) formed in the 2DHS in an in-plane magnetic field $B$. The origin of the spin splitting for holes differs significantly from that for electrons. For bulk holes, the g-factor is defined not only by the constant of coupling of the angular momentum $3/2$ to magnetic field, but also by the Luttinger constants $\gamma_1, \gamma_2$ and $\gamma_3$ defining the heavy and light hole masses. In the high mobility 2DHS, the width of the quantum well (QW) $L$ becomes comparable to the magnetic length $\lambda_B$ for the in-plane $B \sim 3T$. We find that the spin splitting for 2D holes and for holes in QPC is strongly affected by the orbital motion in the presence of the in-plane $B$. We developed the new approach to spectra based on confluent hypergeometric functions. We take into account the anisotropy of the Hamiltonian and calculate the spin splitting for [113] orientation of the 2DHS. For QPC spectra, configurations of in-plane $B$ along and perpendicular to the direction of the current are studied. Our results explain many of the features of spin-resolved QPC conductance observed by Robinson group (PRL, 100, 126401) and by Hamilton group (PRL, 97, 026403). Our analysis also resolves the puzzling red shift of the Fermi energy discovered in optical spectra for QW in-plane magnetic field by Crooker group (Physica E, 22:624).

1:15PM J11.00011 Ferromagnetic vs. Antiferromagnetic Correlations in a Double Dot System, MANAS KULKARNI, Stony Brook University and Brookhaven National Laboratory, ROBERT KONIK, ALEXEI TSVELIK, Brookhaven National Laboratory — We study a double dot system in a parallel geometry using both a large-N diagrammatic and a SBMFT approach. We consider the role of interdot ferromagnetic correlations upon the conduction. We find that at the particle-hole symmetric point that the Friedel sum rule holds and the conduction vanishes. We find that the ground state of the double dot system is a singlet although the correlations between the two dots is primarily ferromagnetic. Hence we observe that the RKKY interaction does not bind the two electrons on the dots into a triplet. We compare our results to a Bethe ansatz analysis of the same system [1]. [1] R.Konik PRL 99, 076602 (2007).
1:27PM J11.00012 Magnetic Splitting of the Zero Bias Peak in a Quantum Point Contact with a Variable Aspect Ratio1. TAI-MIN LIU, BRYAN HEMINGWAY, ANDREI KOGAN, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University, UNIVERSITY OF CINCINNATI TEAM, XAVIER UNIVERSITY COLLABORATION — We have measured the nonlinear conductance of a four-gate Quantum Point Contact (QPC) device fabricated in a GaAs/AlGaAs heterostructure containing a 2-dimensional electron gas. By continuously varying the longitudinal potential profile of the QPC, we controllably create and destroy a local bound state. The nonlinear transport data show both a characteristic Coulomb blockade diamond and a zero-bias peak similar to the Kondo effect signature peak in quantum dots. We find that even when the bound state is suppressed the zero-bias peak persists. Applying an in-plane magnetic field perpendicular to the direction of the current produces a splitting of the peak which closely matches the g-factor data obtained via the cotunneling spectroscopy method in a separate quantum dot on the same chip.

1The research is supported by NSF DMR award No. 0804199 and by University of Cincinnati.

1:39PM J11.00013 Topological spin textures in strongly interacting quantum dots, JORDAN KRYIAKIDIS, CATHERINE J. STEVENSON, Dalhousie University, Halifax, CANADA — We present results of configuration-interaction calculations on two-dimensional quantum dots containing charges with long-range Coulomb repulsion. We focus on correlation-induced spin textures formed at zero magnetic field. By looking at chiral structures, at two- and three-point spin-correlation functions, and at explicit symmetry-breaking fields, a consistent picture emerges of incipient topological spin textures formed throughout the dot and particularly at annular regions of increased electron density. In addition to singular vortex-type structures, 2n-windings are observed in the spin field along these annular regions. These textures are solely due to statistics and repulsion.

1:51PM J11.00014 Spin interference in quantum rings manipulated with quantum point contacts1. FRANCISCO MIRELES, Centro de Nanociencias y Nanotecnología – UNAM, México, LEO DIAGO, Universidad de la Habana, Cuba — The Aharonov-Bohm (AB) and Aharonov-Casher (AC) effects are two well known interference phenomena that may appear in semiconductor quantum rings (QR’s). Although the AB effect has been long observed, its counterpart, the AC effect has been only recently detected in cleaver magnetoconductance oscillations experiments on HgTe/HgCdTe based QR’s exhibiting strong Rashba SO-interaction [1]. In this work, using the S-matrix formalism we study the role of the contacts between the leads and the QR on the AB and AC conductance oscillations of the device in the presence of Rashba and Dresselhaus type of SO interactions. We describe the backscattering and transparency of the conjunctions lead-to-ring through quantum point contacts (QPCs) modelled with gate-controllable saddle-point potentials. The variable transmissivity of the QPCs, adjusted in the experiment by gate voltages and/or applied magnetic fields, is readily incorporated in our approach. It is shown that manipulating electrostatically the confinement strength at the QPCs, may be of utility to implement a novel way to modulate spin interference effects in semiconductor quantum rings. [1] M. König et al., PRL 96, 076804 (2006).

1Work supported in part by DGAPA-UNAM project 1N113-807-3.

2:03PM J11.00015 NGEF Study of the Spontaneous Spin Polarization in a Quantum Point Contact1. JUNJUN WAN, MARC CAHAY, RICHARD NEWROCK, PHILIPPE DEBRAY, University of Cincinnati — A non-equilibrium Green function formalism (NEGF) is used to study the conductance of a side-gated quantum point contact (QPC) in the presence of lateral spin-orbit coupling (LSOC) induced by the electric field due to the gradient of the lateral confining potential. A small asymmetry in the confining potential induced by difference of potential between the two side-gates (SGs) leads to an inversion asymmetry in the LSOC which triggers a spontaneous spin polarization in the QPC. In the regime of single-mode transport, the spontaneous spin polarization can reach nearly 100% when a strong electron-electron (e-e) interaction is taken into account. This leads to the occurrence of a plateau at G = 0.5 (e²/h) in the ballistic conductance without the need of any externally applied magnetic field. Two ingredients are essential for the occurrence of the 0.5 plateau: an asymmetric LSOC and a strong e-e interaction.

1This work is supported by the National Science Foundation under grant ECCS-0725404.


11:15AM J12.00001 Valence band structure in crystalline pentacene thin films1, RICHARD HATCH, DAVID HUBER, HARTMUT HÖCHST, Synchrotron Radiation Center, UW-Madison — Organic semiconductors, such as pentacene (Pn), are beginning to show promise as a low-cost substitute for conventional semiconductors for a variety of electronic devices. The overlap of π-orbitals in the Pn crystal leads to molecular orbital-derived bands. We used angle-resolved photoemission spectroscopy (ARPES) to reveal the Pn in-plane band structure of the two highest occupied molecular orbital-derived bands in crystalline thin film Pn (grown on a Bi substrate) for various temperatures between 75 K and 300 K. We mapped these two bands in several crystallographic directions with special attention given to the region near the top of the valence band and show, within the limits of our experimental resolution, that temperature does not change the dispersions of these bands. We fit the band structure to a tight binding model and compared our results with recent theoretical predictions[1-2]. We also calculated the in-plane reciprocal effective mass for the M point and compared it with the measured mobility. [1] H. Yoshida et. al. Phys. Rev. B 77, 235205 (2008). [2] G. A. de Wijs et. al. Synth. Met. 139, 109 (2003).

1This work is based upon research conducted at the Synchrotron Radiation Center, University of Wisconsin-Madison, which is supported by the NSF under Award No. DMR-0537588

11:27AM J12.00002 The growth mechanism of anisotropic organic molecular films, A. AL-MAHBOOB, WPI-Advanced Institute for Materials Research, Tohoku University, Y. FUJIKAWA, Institute for Materials Research, Tohoku University, J.T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, QIKUN XUE, T. SAKURAI, WPI-Advanced Institute for Materials Research, Tohoku University — The anisotropy in molecular structure and crystal packing may complicate nucleation and growth processes in organic molecular films. The growth mechanism of pentacene (Pn) films has been studied by real time low-energy electron microscopy. Pn is most promising for FET application as it shows the highest field-effect mobility among organic thin-films. We observed delayed nucleation and formation of large grains (as large as 0.5 mm in diameter) on semiconducting α/3-Bi-Si(111) and on semi-metallic Bi(0001)/Si(111), with a significant delay in film growth after stopping Pn deposition, indicating long diffusion time. This is in contrast to the growth of Pn on SAMs, oxides or wetting layer on clean silicon surfaces. The long diffusion time could be explained by large barrier for Pn nucleation with standing-up orientation from a lying-down diffusing state due to stronger interaction between lying molecules and Bi-treated substrates.
11:39AM J12.00003 Morphology and Crystalline Structure of the Epitaxial Growth of Tetracene Thin Films on H/Si(001)-2x1 Substrate \cite{1}, ANDREW TERSIGNI, DE-TONG JIANG, XIAORONG QIN, Dept. of Physics, University of Guelph — Epitaxial growth of tetracene films on H/Si(001)-2x1 surface has been studied systematically using AFM, STM and X-ray diffraction. The surface morphology and in-plane lattice structure observed from AFM and STM are compared with that extracted from the diffraction measurements to reach a consistent description on the in-plane and out-plane lattice parameters of different epitaxial domains, respectively. The influence of the substrate roughness and film coverage to the morphology and underlying lattice structures will be discussed in the light of various characteristics revealed by the multiple structural tools.

1 NSERC Canada

11:51AM J12.00004 Structural investigation of pentacene on Ag(111) by density functional theory \cite{2}, FATIH DANISMAN, Middle East Technical University, ERSEN METE, Balikesir University, SINASI ELLIAALTIĞGLU, Middle East Technical University — We have used density functional theory (DFT) calculations based on the projector augmented wave (PAW) method to investigate the initial growth patterns of pentacene (C_{22}H_{14}) on Ag(111) surface. Here we will report our initial findings and provide a discussion of the results from the point of view of our previous experimental findings. Pentacene prefers to stay planar on Ag(111) surface and aligns perfectly along lattice vector (1,-1,0) without any molecular deformation at a height of 3.74 Å. At 1 ML coverage the separation between the molecular layer and the surface plane extends to 4.14 Å due to intermolecular interactions weakening surface-pentacene attraction. While the first ML remains flat, the molecules on a second full pentacene layer rearrange in a herringbone fashion which is energetically slightly more preferable when compared with a second layer composed of flat lying molecules. With addition of third and fourth layers pentacene molecules continue to maintain the herringbone configuration, with the stability of the herringbone configuration relative to the flat one increasing to 0.13 eV for the 3 ML film, while the first ML always remains flat. Therefore, our calculations indicate bulk-like initial stages for the growth pattern.

12:03PM J12.00005 Magnetic and structural behaviors of transitional metallo-porphines monolayer and bilayer on Ag(111) \cite{3}, Q.X. TIAN, J.B. XU, DEPT OF ELEC ENGI AND MSRC, THE CHINESE UNIVERSITY OF HONG KONG TEAM, CHEMISTRY DEPT, PRINCETON UNIVERSITY COLLABORATION — Five monolayers and bilayers of transitional metallo-porphine(MP) (Mn, Fe, Co, Ni, Cu) on Ag(111) substrate are investigated by ab initio calculation. The strong coupling of FeP and CoP MP/Ag(111) interface leads to magnetic-nonmagnetic transition. The competition mechanism between intermolecular ferromagnetic exchange interaction and coupling of FeP/Ag(111) prevents the magnetic-nonmagnetic transition of interface. The top layer of all 5 bilayers keeps its intrinsic magnetic properties and planar structures, so the bottom layer of the bilayer serves the role of buffer layer. These theoretical results could be used to explain the recent STM and XPS experiments. A new interfacial magnetic competition mechanism has been proposed and hopefully it will influence the construction and design of future molecular spintronics.

12:15PM J12.00006 Quantitative Grain Size Distributions of Magnetic Organic Thin Films \cite{4}, THOMAS GREDIG, K. PAUL GENTRY, California State University Long Beach, IVAN K. SCHULLER, University of California San Diego — Many electronic, optical, and magnetic properties of organic thin films depend on the precise morphology of grains. Quantitative grain size distributions of an asymmetric organic molecule are presented and correlated with the magnetic characteristics. Iron phthalocyanine (FePc) thin films are grown on sapphire substrates at varied deposition temperatures to study the effect of grain growth and to experimentally quantify the grain size distributions in organic thin films based on atomic force microscopy images. The data of over 3000 grains for each sample show a pronounced asymmetric growth of grains from a spherical to an elongated needle-like shape. The size along the major axes increases from 35nm to 200nm and is distributed in a different way than the minor axes, which grow from 25nm to 90nm. The dissimilar distributions are attributed to an asymmetric growth rate. Low-temperature hysteresis loops and temperature-dependent magnetization curves for these FePc thin films illustrate the effect of the length of quasi one-dimensional Fe chains on the magnetic properties.

1 This work was supported by a SCAC award, start-up fund from the CNSM at California State University, Long Beach and AFOSR.

12:27PM J12.00007 The structure of the C_{60} monolayer on Pb(111) \cite{5}, HSIN-I LI, Physics Department, Penn State University, KATHARINA FRANKE, JOSE PASCUAL, Institut fuer Experimentalphysik. Freie Universitaet Berlin, RENEE DIEHL, Physics Department, Penn State University, LEED, PHYSICS DEPARTMENT, PENN STATE UNIVERSITY TEAM, STM, INSTITUT FUER EXPERIMENTALPHYSIK, FREIE UNIVERSITAT BERLIN TEAM — Low-energy electron diffraction and scanning tunneling microscopy studies indicate that a monolayer of C_{60} on Pb(111) forms a modulated structure having an average C_{22}H_{14} nearest-neighbor distance of about 10Å, but a period of about 46Å. The data were analyzed in the context of the Tkatchenko method \cite{6}, and the monolayer structure was identified as two coexisting higher-order commensurate structures, namely (√169 x √169)R16.90° and (√169 x √169)R21.31°, both with 21 C_{60} molecules and 169 Pb atoms in their unit cells. This modulated structure has implications for the electronic structure of the C_{60} film, as measured using scanning tunneling spectroscopy.


3 This research is supported by NSF-DMR-0505160.

12:39PM J12.00008 The structures of a C_{60} monolayer on Al(111) \cite{7}, HEEKEUN SHIN, HSIN-I LI, The Pennsylvania State University, KATARIINA PUSSI, Lappeenranta university of technology, RENEE DIEHL, The Pennsylvania State University — The interfaces of C_{60} films with metal surfaces are of particular interest for molecular electronics applications. The electronic properties of these films are known to depend strongly on their structures and the relative molecular orientations of the C_{60} molecules, yet there are few detailed structure determinations for C_{60} films. When grown at room temperature, C_{60} on Al(111) forms a (2/3×2/3×1)R30° structure with one C_{60} molecule per unit cell, which upon heating converts to a 6x6 structure with 3 C_{60} molecules per unit cell. We present a LEED study of the transition between these structures, a LEED I(E) analysis of the 6x6 structure, and characterization of the adsorption of rare gases onto the surface of the 6x6 C_{60} film. This research is supported by NSF-DMR-0505160 and the Academy of Finland.
The adsorption of C_{60} fullerene molecules on Nanostructured Au (111)  

XIN ZHANG, QUANMIN GUO, RICHARD PALMER, University of Birmingham, NANOSCALE PHYSICS RESEARCH LABORATORY TEAM — The monolayer growth of C_{60} molecules on the Au (111) surface has been studied using STM in ultra high vacuum. The C_{60} molecules tend to form close-packed layers due to a strong inter-molecular interaction. However, within the close-packed layer, there are finer, secondary structures that are specific to each of the three C_{60}/Au interfacial structures (2√3×√3,R30°, in-phase (R0°) and R14°) observed [1]. This is a consequence of the molecule-substrate interaction and our findings demonstrate a much more complex structural variation at the molecule-substrate interface than previously assumed. Furthermore, within the R14° C_{60} layer, slightly darker molecules (30 pm lower) aligned along the 311-20 direction with a ~6 nm spacing are observed and these molecules are arranged in a reasonably well-ordered two-dimensional lattice. C_{60} molecules are also found to decorate the elbow sites of the herringbone reconstructed Au(111) even at room, and when fullerences are deposited to arrays of fabricated monolayer gold stripes (gold-fingers) [2], the molecules show step-specific attachment where the step edges with the (111) micro-facet are preferentially populated.

Tuesday, March 17, 2009 11:15 AM - 2:15 PM –
Session J13 DCOMP: Numerical Methods for Strongly Correlated Systems: Hubbard and
Quasi-Particle 309

11:15AM J13.00001 Evaluation of time-resolved photoemission spectra from nonequilibrium,
time-domain Green functions, B. MORITZ, T. P. DEVEREAUX, SLAC and Stanford University, H. R. KRISHNAMURTHY, Indian Institute of
Science, J. K. FREERICKS, Georgetown University — Recent experiments have shown the power of femtosecond time-resolved, pump-probe photoelectron
spectroscopy to probe, directly, the nonequilibrium, real-time dynamics of excitations in a correlated material. We use nonequilibrium dynamical mean-field
theory to study the spinless Falicov-Kimball model driven (pumped) out of equilibrium by a constant electric field turned on at \( t = 0 \). We demonstrate the
proper evaluation of the time-resolved photoemission intensity as a function of pump-probe delay for both metallic and Mott-insulating phases of the model
and the dependence of the intensity profile on the specific details of the probe pulse’s lineshape and duration.

11:27AM J13.00002 Mott-like behavior in the pseudogap region of the Hubbard model(1), DIM-
ITRIOS GALANAKIS, Louisiana State Univ., KARLIS MIKELSONS, EHSAN KHATAMI, MARK JARRELL, Louisiana State Univ. and Univ. of Cincinnati,
ALEXANDRU MACRIDIN, MICHAEL MA, Univ. of Cincinnati, JUANA MORENO, Louisiana State Univ. — We study the phase diagram of the two-dimensional
Hubbard model using the Dynamical Cluster Approximation (DCA) in conjunction with the weak-coupling continuous time quantum Monte Carlo (CTQMC) as
the cluster solver. We verify the existence of a quantum critical point at a finite electron doping which separates a fermi liquid region at low electron doping
from the pseudogap region at high electron doping(2). In the pseudogap region the double occupancy, the two particle correlation functions and spectra reveal
a synergism between the development of momenstate and the appearance of short ranged order. We discuss the connection between our results and experiments.

3This work was supported by the National Science Foundation through OISE-0730290, DMR-0548011, and DMR-0706379.
3Vidhyadhiraja et. al., arXiv:0809.1477v1

11:39AM J13.00003 Pairing instabilities and Bose condensation in Hubbard nanoclusters , GAYANATH FERNANDO, KALUM PALANDAGE, Department of Physics, University of Connecticut, Storrs, ARMEN KOCHARIAN, Department of Physics,
California State University, Los Angeles, JAMES DAVENPORT, Computational Science Center, Brookhaven National Laboratory, Upton — Pairing instabilities
found from exact studies of small Hubbard clusters with different topologies appear to provide answers to some long standing puzzles. Electronic charge and spin
pairing instabilities in a phase space defined by temperature, magnetic field and chemical potential, lead to properties that are remarkably similar to correlated,
inhomogeneous bulk systems such as the high temperature superconductors and colossal magnetoresistance materials. In particular, the role of square- planar
graphene is geometry born out as the vertex coupling in an octahedron is shown to have a detrimental effect on the negative charge and positive spin gaps, which are
favorable to forming a Bose condensate in the region of instability. In addition, it is shown that magnetic flux can get trapped in stable minima at half integral
units of the flux quantum.

11:51AM J13.00004 Functional renormalization group beyond the static approximation and
its application to two-dimensional Hubbard model, HIROKAZU TAKASHIMA, University of Tokyo, Dept. Phys., RYOTARO
ARITA, University of Tokyo, Dept. Applied Phys., KAZUHIKO KUROI KUROI, University of Electro-Communications, HIDEO AOKI, University of Tokyo, Dept. Phys.
— While the functional renormalization group(1RG) is a powerful theoretical method for strongly correlated electron systems which treats diagrams systematically
within a framework of quantum field theory, the static approximation is adopted where the Matsubara frequency dependence of the four-point coupling and renormalization
for the self-energy are ignored. Here we propose a method to go beyond the static approximation by devising an efficient parameterization for the
four-point coupling in the Matsubara frequency space, which is combined with a previous improved algorithm of ours(1) based on a Cartesian box discretization.

12:03PM J13.00005 Parquet approximation calculation for the 2D Hubbard model(1) , SHUXIANG
YANG, HERBERT FOTSO, JUN LIU, MARK JARRELL, University of Cincinnati, EDUARDO D’AZEVEDO, THOMAS MAIER, Oak Ridge National Laboratory,
KAREN TOMKO, Ohio Supercomputer Center, RICHARD SCALETTAR, University of California - Davis, THOMAS PRUSCHKE, University of Goettingen,
Germany — We present a numerical solution of the parquet approximation on a half-filled 4x4 Hubbard cluster. The parquet formalism is a two-particle self
consistent set of equations relating the reducible, irreducible, and fully irreducible vertexes. The simplest approximation from this formalism is the so-called
parquet approximation, in which the fully irreducible vertex is approximated by the bare interaction. Our results are compared with results from Self-Consistent
2nd-order approximation, Fluctuation Exchange (FLEX) approximation and the Determinental Quantum Monte Carlo (DQMC) calculation.

3We would like to acknowledge the support from SciDAC and NSF PIRE

12:15PM J13.00006 Spatially inhomogeneous phase in the two-dimensional repulsive Hubbard
model(1), CHIA-CHEN CHANG, SHIWEI ZHANG, Department of Physics, The College of William and Mary — Using recent advances in the constrained-
path auxiliary-field quantum Monte Carlo method, we study the ground state of the two-dimensional, single-band Hubbard model at intermediate interactions
\( (2 < U/J \leq 4) \). In the first part of this study, we have determined the equation of state and also calculated the spin-spin correlation functions in square
lattices up to size 16 x 16. Shell effects are eliminated and finite-size effects are greatly reduced by boundary condition integration. It was shown that, upon
doping, the system separates into a region with antiferromagnetic (AF) order and a hole-containing region without AF order. In the second part, we study
rectangular supercells up to 8 x 64 to examine the nature of this inhomogeneous phase, in particular to probe phase separation versus stripes and spin-density
12:27PM J13.00007 Inhomogeneous ground state in the Hubbard model: a mean-field study. JIE XU, CHIA-CHEN CHANG, ERIC J. WALTER, SHIWEI ZHANG, The College of William and Mary — We report unrestricted Hartree-Fock (UHF) results for the ground state of the single-band Hubbard model in two- and three-dimensions with repulsive onsite interaction and nearest-neighbor hopping. At half-filling, the Hartree-Fock (HF) approach is sufficient to capture the basic physics of long-range antiferromagnetic order. Away from half-filling, many earlier HF calculations have been performed in the 2-D Hubbard model, which indicated the formation of domain walls and stripes. We numerically solve the self-consistent UHF equations for a range of densities at weak and intermediate interaction strengths. An annealing scheme coupled with multiple initial configurations is adopted to reach the global minimum. Our goal is to contrast the UHF ground state in the Hubbard model and the HF spin-density wave states in the continuum (jellium) [1]. A second goal is to obtain quantitative information of the UHF ground state for examination by accurate many-body methods such as quantum Monte Carlo. [1] A. W. Overhauser, Phys. Rev. 128, 1437 (1962); Shiwei Zhang and D.M.Ceperley, Phys. Rev. Lett. 100, 236404 (2008).

1Supported by NSF and ARO

12:39PM J13.00008 Discontinuous quenching of quasi-particle states in nonequilibrium dynamical mean-field theory. RYAN HEARY, JONG HAN, SUNY at Buffalo — In an effort to model strongly correlated heterojunctions in nonequilibrium we construct a nonequilibrium dynamical mean-field theory for the Hubbard model where each lattice site is a superposition of a left-moving and right-moving state. The left and right movers have the respective chemical potentials, \( \mu_L = \frac{\Phi}{2} \) and \( \mu_R = -\frac{\Phi}{2} \), where \( \Phi \) is the chemical potential bias. The quasi-particle properties are calculated as a function of the Coulomb interaction, \( U \), and \( \Phi \). As the chemical potential bias is turned on we find that the quasi-particles become strongly renormalized. When \( U_{ij} < U < U\mu \), where \( U\mu \) is the critical \( U \) for the metal-insulator transition in equilibrium and \( U_{ij} \sim 0.7U\mu \). the quasi-particles are destroyed discontinuously at a critical chemical potential bias, \( \Phi_{\text{crit}} \). For \( U < U_{ij} \) the quasi-particles disappear continuously as \( \Phi \) is enhanced. Therefore \( U_{ij} \) is the critical \( U \) which defines the boundary between the quasi-particles being continuously and discontinuously suppressed. By defining the quasi-particle energy, \( \epsilon_{QP} \), as the half-width at half-maximum of the quasi-particle peak, we find that for \( \Phi/\Phi_{\text{crit}} \leq 0.4 \), the quasi-particle energies scale to a single curve.

1Supported by NSF DMR-0426826

12:51PM J13.00009 Self-consistent solution for the Hubbard model at the two-particle and one-particle level using the parquet formalism. HERBERT FOTSO, SHUXIANG YANG, JUN LIU, MARK JARRELL, University of Cincinnati, EDUARDO D’AZEVEDO, THOMAS MAIER, Oak Ridge National Laboratory, KAREN TOMKO, Ohio Supercomputer Center, RICHARD SCALLETAR, University of California - Davis — The parquet formalism is used to solve self-consistently, both at the one-particle and at the two-particle levels, the Hubbard model on a 2-D square lattice. The parquet equation and the Bethe-Salpeter equation are combined into one Newton fixed point problem which is then solved by taking advantage of the existing linear solvers such as GMRES and BiCGStab. Some quantities of interest are calculated and the results are compared to those of Determinental Quantum Monte Carlo (DQMC). We also discuss the importance of this work in the multiscale treatment of the High Tc Cuprates.

1We would like to acknowledge support from SciDAC and NSF PIRE

1:03PM J13.00010 Quantum Monte Carlo study of few-electron concentric double quantum rings. LEONARDO COLLETTI, Istituto Nazionale di Fisica Nucleare, Italy, FRANCESC MALET, MARTI PI, Universitat de Barcelona, Spain, FRANCESCO PEDERIVA, Università di Trento, Italy — We consider few-electron concentric double quantum rings with parabolic confining potential and compare the ground-state energies calculated by exact diagonalization of the Hamiltonian, accurate quantum Monte Carlo and local spin-density functional approaches. Electronic localization in one of the rings and the formation of rotating Wigner molecules is shown respectively from the one-body and the two-body density operators. As the confinement strength is finely increased, the circularly-symmetric electron density exhibits a radial crossover from the outer ring to the inner one without altering the angular character of the system.

1:15PM J13.00011 Accurate Determination of Tensor Network State of Quantum Lattice Models in Two Dimensions. TAO XIANG, H.C. JIANG, Z.Y. XIE, Q.N. CHEN, Z.Y. WENG, Institute of Physics, Chinese Academy of Sciences — We have proposed a novel numerical method to calculate accurately physical quantities of the ground state using the tensor network wave function in two dimensions. The tensor network wave function is determined by an iterative projection approach which uses the Trotter-Suzuki decomposition formula of quantum operators and the singular value decomposition of matrix. The norm of the wave function and the expectation value of a physical observable are evaluated by a novel second renormalization group method of tensors. Our method allows a tensor network wave function with a high bond degree of freedom to be handled accurately and efficiently in the thermodynamic limit. For the Heisenberg model on a honeycomb or square lattice, our results for the ground state energy and the staggered magnetization agree well with those obtained by the quantum Monte Carlo and other approaches.

1:27PM J13.00012 ABSTRACT WITHDRAWN

1:39PM J13.00013 Electronic structure of LaM\(_{2}\)O\(_{3}\) (M=Ti~Cu) by GW approximation. YOSHIRO NOHARA, TAKEO FUJIWARA, University of Tokyo — We investigate the electronic structure of LaM\(_{2}\)O\(_{3}\) (M=Ti~Cu) by GW approximation. The calculated spectra show good agreement with the experimentally observed ones. The on-site Coulomb interaction is affected by strong screening mechanism in trivalent transition metal ions, which is qualitatively different from those in mono-oxides M\O\(_{3}\) of divalent transition metals. In trivalent transition metal ion systems LaM\(_{2}\)O\(_{3}\), 3d electrons are affected by deep atomic potential. Therefore, the 3d orbital locates energetically much nearer to O 2p levels than in M\O\(_{3}\). Moreover, in the cases of M\(^{++}\)=C\(_{2}\)\(^{2+}\), M\(^{++}\)=Mn\(_{2}\)\(^{4+}\) and Fe\(_{2}\)\(^{3+}\) systems, transition metal ions are well spin-polarized, and 3d levels locate very near to O 2p levels. As a result, these systems have large screening effects due to the extended d-electrons. In the cases of M\(^{++}\)=Ni\(_{2}\)\(^{2+}\) and Cu\(_{2}\)\(^{2+}\), the systems are metallic and are affected by strong screening effects. In the other cases of M\(^{++}\)=Ti\(_{2}\)\(^{4+}\), V\(_{2}\)\(^{4+}\), and Co\(_{2}\)\(^{3+}\), there are small screening effects causing large static screened Coulomb interaction.

1:51PM J13.00014 GW correlation effects on the quasiparticle energies of Np and Pu. ATHANASIOS CHANTIS, ROBERT ALBERS, Theoretical Division, Los Alamos National Laboratory, AXEL SVANE, NIELS CHRISTENSEN, Department of Physics and Astronomy, University of Aarhus, MARK VAN SCHILFGAARDE, TAKAO KOTANI, School of Materials, Arizona State University — We present results for the electronic structure of plutonium and neptunium by using a recently developed quasiparticle self-consistent GW method (QSGW). The self-consistent GW quasiparticle energies are compared to those obtained within the Local Density Approximation (LDA) for several volumes of the unit cell. The goal of the calculations is to understand systematic trends in the effects of electronic correlations on the quasiparticle energy bands as a function of the localization of the f orbitals. We show that correlation effects narrow the f bands in two significantly different ways. Besides the expected narrowing of individual f bands (flatter dispersion), we find that an even more significant effect on the f bands is a decrease in the crystal-field splitting of the different bands. We discuss how these changes affect the topology of the Fermi surface and we demonstrate the importance of the quasiparticle self-consistency in obtaining these results.
Porosity of mixed granular media of hard and soft grains. EMILIE VERNEUIL, DOUGLAS J. DURIAN, University of Pennsylvania — The addition of soft particles to granular media modifies the packing properties such as the volume fraction and the interconnection of pores as a consequence of the particles squishiness. A macroscopic property that depends on the local arrangement of the grains is the hydraulic conductivity. Hence, hydrogen particle disks are developed as additives to sandy soils to improve the irrigation efficiency by decreasing the rate of far depth infiltration. However, the parameters that control the mixed material porosity have not been explored. Our experimental study of the flow properties of mixtures of glass beads and swollen hydrogels aims at deriving simple arguments to connect the macro-scale measurement of the hydraulic conductivity to the arrangement of the grains around the soft particles, which determines the fraction of blocked pores. Our results show that the porosity decreases with the number of swollen gel per unit volume of the mixture. The conductivity also decreases as the size ratio of gel to glass bead decreases down to 1. A simple description accounting for the elastic contacts between glass beads and gel surface qualitatively accounts for the data.

Experimental characterization of microstate probabilities in mechanically stable packing of frictionless disks. M.D. SHATTUCK, Levich Institute and Physics Department, The City College of New York, New York, NY, G.-J. GAO, Department of Mechanical Engineering, Yale University, New Haven, CT, J. BLAWZDIEWICZ, C.S. O’HERN, Departments of Mechanical Engineering and Physics, Yale University, New Haven, CT — We report on a new experimental technique to produce mechanically stable packings of frictionless disks. The system consists of a quasi-2D vertical cell filled with bi-disperse disks. The disks are vigorously shaken and then allowed to settle under gravity in the presence of high-frequency low-amplitude vibrations to eliminate frictional effects. For a system of 7 particles we find approximately 1000 mechanically stable states. The most probable states occur at least 10^6 times more often than those that are least probable. This is in direct contradiction to the fundamental postulate in statistical mechanics, that all possible microstates are equally probable and calls into question granular theories based on this assumption. We have measured the frequency distribution of the states in the systems and in corresponding discrete element simulations, and find excellent agreement. We have also examined how the microstate distribution scales with system size and will connect the microstates to macroscopic quantities such as the density to predict the statistics of macroscopic properties.

Spectral responses in granular compaction. LING-NAN ZOU, The James Franck Institute and Department of Physics, the University of Chicago — I study the compaction of a granular pack under periodic tapping. The magnitude of acceleration \( \Gamma \) at each tap is modulated with frequency \( \omega \) and amplitude \( \delta \): \( \Gamma(t) = \Gamma_{DC} + \Gamma \sin(\omega t) \), where \( t \) is time measured by the number of taps. From the temporal modulation \( \delta v \) in packing volume \( v \), frequency-locked to the modulated tapping input, we can define the real and imaginary volume susceptibilities \( 
\chi'_\nu(t) = (\delta v / \delta \Gamma) \cos \theta \) and \( 
\chi''_\nu(t) = (\delta v / \delta \Gamma) \sin \theta \), where \( \theta \) is the phase lag between \( \Gamma(t) \) and \( \nu(t) \). As a function of \( \Gamma_{DC} \), \( \chi'_\nu \) and \( \chi''_\nu \) are peaked at low \( \Gamma_{DC} \), a behavior reminiscent of the temperature-dependent susceptibilities in dielectric and spin glasses. For the packing of small particles (\( d = 0.5 \text{ mm} \)) in ambient pressure, \( \chi'_\nu \) exhibits memory and rejuvenation effects under \( \Gamma_{DC} \) cycling, similar to that seen in the magnetic susceptibility of spin glasses when subjected to thermal cycling \( [1] \). However this memory effect is suppressed for the packing of larger particles and in vacuum. The measurement of volume susceptibilities shows promise as a new way to study the packing of granular materials, and as an avenue to explore analogies between jammed grains and molecular and spin glasses.


Deformed Droplets in Static Two-Dimensional Emulsions. PEARL J. YOUNG, DANDAN CHEN, ERIC R. WEEKES, Physics Dept., Emory University — We confine oil-in-water emulsions between two parallel plates, so that the droplets are essentially squeezed into quasi two-dimensional disks, somewhat analogous to granular photoelastic disks. By varying droplet area fraction, we seek to quantify the jamming transition of this static system. At a critical area fraction, the composition of the system should no longer be characterized primarily by circular disks but by disks deformed to varying degrees. We study a system of toluene droplets in water. As expected, we find that an increase in area fraction corresponds with an increase in average droplet deformation. Further, an increase in average droplet deformation corresponds with an increase in the heterogeneity of deformity within a given sample.

Jammed Rod-like Granular Materials in Hoppers. SUMMER SARAF, SCOTT FRANKLIN, Rochester Institute of Technology — Long thin rods form solid plugs that are far more rigid than piles of ordinary sand, greatly affecting their ability to flow through small openings. We have built a hopper whose aperture, angle, and width can be independently varied and are studying the frequency with which rods of different length, width, and aspect ratio jam. As the opening aperture becomes larger, the mean number of particles that exit the hopper before a jam occurs naturally increases, but the probability distribution of fluctuations about this mean is unchanged. Unexpectedly, whereas the event distribution function \( P(s) \) for spheres decays exponentially, we find the distribution for rods falls off as a power law with exponent \( \alpha = -1.41 \pm 0.08 \). We are also investigating the growth of the mean event size \( \langle s \rangle \), as the aperture increases for possible divergence, which would imply a critical aperture size above which particles would never jam.

Forces and displacements near the granular jamming threshold. MAHESH BANDI, Los Alamos National Laboratory, ANDRAS LIBAL, University of Antwerp, MICHAEL RIVERA, ROBERT ECKE, Los Alamos National Laboratory — We experimentally study the dynamics of jamming by dragging a probe disk in a two-dimensional bi-dispersed system of randomly packed photo-elastic disks. All measurements are made at packing fractions relative to the critical fraction at which jamming occurs. We measure the local force felt by the probe disk and compare it with the system’s global response with sensors placed along the system boundaries. We also visually monitor the disk displacements in the system, which are expected to become increasingly constrained as a function of increasing packing fraction.
12:27PM J14.00007 The angoricity describes the approach to the jamming , KUN WANG, CHAOMING SONG, PING WANG, HERNAN MAKSE, Levich Institute and Physics Department of CCNY — The application of concepts from equilibrium statistical mechanics to out of equilibrium systems has a long history offering the fascinating possibility to describe a diverse range of systems from glasses to grains. For jammed systems, the key idea was to replace the energy ensemble describing conservative systems by the volume ensemble for dissipative jammed systems. However, this approach is not able to describe the jamming critical point for deformable particles such as emulsions where the volume fraction, coordination number and elastic moduli behaves as power-law of the external stress as the system approaches jamming. The geometrical considerations to be augmented by the ensemble of stresses described by the angoricity which replaces the role played by the temperature in thermal systems. Here we perform a basic test of the stress ensemble of jammed matter by following two independent approaches: we exhaustively enumerate the available jammed states and numerically follow the dynamics of the system near the jamming point. A direct comparison between both methods supports the idea of thermalization at a given angoricity which is shown to determine the systems state as it approaches the jamming transition. This result opens the possibility to calculate important quantities near J-point.

12:39PM J14.00008 Equilibration in model granular subsystems: An experimental test for Edwards’ compactivity , FREDERIC LECHENAULT, JAMES PUCKETT, KAREN DANIELS, NCSU — We experimentally investigate the statistical features of the stationary states reached by two idealized granular liquids able to exchange volume. The system consists in two binary mixtures of the same number (and area) of soft disks, but with different surface properties. The disks sit on a horizontal air table and are separated by a mobile wall. Energy is injected in the system by means of an array of randomly activated coil bumpers standing as the edges of the cell. Due to the energy injection, the system acts like a slow liquid and eventually jams at high packing fraction. We characterize the macroscopic states by studying the motion of the piston. We find that its average position is different from one half, and is a non monotonic function of the overall packing fraction, which reveals the crucial role played by the surface properties in the corresponding density of states. We then study the bulk statistics of the packing fraction and find confirmation of the macroscopic behavior. However, the local fluctuations of the packing fraction are uniquely determined by its average, and hence independent of the interaction between disks. This result, together with the existence of a point at which the two sub-systems have the same volume, enables us to show that Edwards’ compactivity does not have the same value in the two equilibrated subsystems.

12:51PM J14.00009 Stability of Packings of Soft Elliptical Grains in 2D1 , MITCHELL MAILMAN, BULBUL CHAKRABORTY, Brandeis University, CARL SCHRECK, COREY O’HERN, Yale University — Simulations of hard ellipses packings show that these ellipse packings are generally hypostatic. By using a dynamical matrix approach to analyzing the stability of two-dimensional ellipse packings, we show that the degree of hypostaticity is related to the fraction of zero-frequency modes. The packings are generated using a compression protocol previously employed in disk packings and an energy function based on the overlap model developed by Perram and Wertheim. The density of states exhibits a low frequency peak that approaches zero as the compression is reduced. There is a gap separating this peak from the higher frequency modes. In this talk, we will demonstrate the existence of a scaling relation between the vibrational spectra at different aspect ratios. We will also discuss the origin of the low frequency modes and the origin of the scaling. Analysis of the relationship between contact numbers and vibrational modes will be used to compare and contrast the jamming transition in disks and ellipses.

1The work of MM and BC has been supported by NSF DMR-0549762 and The work of CS and CO has been supported by CDI-0835742 (CS) and DMR-0448838 (CSO).

1:03PM J14.00010 Shearing dynamics and jamming density , PETER OLSSON, DANIEL VÄGBERG, Department of Physics, Umeå University, Umeå, Sweden, STEPHEN TIETEL, Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627 — We study the effect of a shearing dynamics on the properties of a granular system, by examining how the jamming density depends on the preparation of the starting configurations. Whereas the jamming density at point J was obtained by relaxing random configurations [O’Hern et al, Phys. Rev. E 68, 011306 (2003)], we apply this method to configurations obtained after shearing the system at a certain shear rate. We find that the jamming density increases somewhat and that this effect is more pronounced for configurations produced at smaller shear rates. Different measures of the order of the jammed configurations are also discussed.

1:15PM J14.00011 Theory of Elasticity and Glassy Dynamics of Suspensions of Soft Particles , JIAN YANG, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — A microscopic theory for the shear modulus and slow dynamics of soft colloidal systems composed of many arm star-polymers and intra-molecularly crosslinked microgels is described. The role of particle volume fraction and softness (arm number for stars and contact modulus for micropel grains) on the ideal mode coupling kinetic arrest transition, elastic modulus, relaxation time in the activated hopping regime, diffusion constant, dynamic fragility, and absolute yield stress and strain have been systematically explored. The low-frequency shear modulus is characterized by two volume fraction regimes: power law scaling at intermediate volume fractions and a linear law beyond the nominal jamming point. Connections between single particle softenes, interparticle packing correlations, and viscoelastic properties have been established. For both microgels and many arm stars, the effective dynamical fragility varies over a wide range as a function of particle softness. Comparisons of the theoretical results with experiments on many arm star and microgel paste systems have been carried out.

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J15 GQI: Quantum Entanglement 316

11:15AM J15.00001 Understanding Entanglement as a Resource for Quantum Information Processing2 , SCOTT M. COHEN, Department of Physics, Duquesne University — Ever since Erwin Schrodinger shocked the physics world by killing (and not killing) his cat, entanglement has played a critical role in attempts to understand quantum mechanics. More recently, entanglement has been shown to be a valuable resource, of central importance for quantum computation and the processing of quantum information. In this talk, I will describe a new diagrammatic approach to under-standing why entanglement is so valuable, the key idea being that the eglement between two systems “creates” multiple images of the state of a third. By way of example, I will show how to “visualize” teleportation of unknown quantum states, and how to use entanglement to determine the (unknown) state of a spatially distributed, multipartite quantum system. Illustirative examples of this entanglement-assisted local state discrimination are sets of orthogonal product states exhibiting what is known as “non-locality without entanglement”, including unextendible product bases. These ideas have also proven useful in using entanglement to implement a unitary interaction between spatially separated (and therefore non-interacting!) systems.

2Supported in part by NSF Grant PHY-0456951 and PHY-0757251 and through a grant from the Research Corporation.
the same central charge. Interpretations of the results are given in terms of branch-point twist fields. The present study provides a new way to show that the information is scale-invariant and depends on the compactification radius (or the Tomonaga-Luttinger parameter) of the bosonic field, as opposed to the general prediction of Calabrese and Cardy. Furthermore, we show that states known as the maximal slice states always violate the Svetlichny inequality and analogous to the 2-qubit case, the amount of violation increases with the 3-tangle. The generalized GHZ states and the maximal slice states have unique tripartite entanglement and nonlocality properties in the set of all pure states.

Quantum Noise as an Entanglement Entropy Meter.

We investigate the generic scaling of the mutual information in a class of one-dimensional quantum critical systems described by a bosonic field theory with a central charge $c=1$, and show that it is universal. A numerical analysis of a spin-chain model reveals that the mutual informations have unique tripartite entanglement and nonlocality properties in the set of all pure states. The present study provides a new way to determine the compactification radius, and furthermore demonstrates the ability of the mutual information to distinguish different conformal field theories with the same central charge.

Genuine tripartite entanglement and nonlocality in 3-qubit GHZ-class states.

SHOHINI GHOSE, NEIL SINCLAIR, SHANTANU DEBNATH, Wilfrid Laurier University. RENE STOCK, University of Toronto. PRANAW RUNGTA, IIS, India — Multiqubit entanglement is a crucial ingredient for large-scale quantum information processing, and has been the focus of several recent studies. Entanglement between qubits can lead to violations of Bell-type inequalities that are satisfied by local hidden variable models, indicating the nonlocal nature of the correlations between qubits. For 2-qubit pure states, bipartite entanglement is simply related to the Bell-CHSH nonlocality parameter. No such analytical relation between multipartite entanglement and nonlocality has yet been obtained for systems of three or more qubits. We have derived relationships between genuine tripartite entanglement and nonlocality for families of 3-qubit GHZ-class pure states. We quantify tripartite entanglement by the 3-tangle and derive its relationship to the Svetlichny inequality for testing tripartite nonlocality. For the class of generalized GHZ states, although the 3-tangle is always non-zero, we identify some states that do not violate the Svetlichny inequality. Furthermore, we show that states known as the maximal slice states always violate the Svetlichny inequality and analogous to the 2-qubit case, the amount of violation increases with the 3-tangle. The generalized GHZ states and the maximal slice states have unique tripartite entanglement and nonlocality properties in the set of all pure states.

Coherent Light Fields for Entanglement based Quantum Communication.

KIM FOOK LEE, Department of Physics, Michigan Technological University, Houghton, MI 49931 — Nonlocal polarization correlations of two distant observers based on Stapp's formulation are observed by using coherent light fields. Using a 50/50 beam splitter transformation, a vertically polarized coherent light field is entangled with a horizontally polarized coherent noise field. The superposed light fields at each output port of the beam splitter are sent to two distant observers, where the fields are interfered and manipulated at each observer by using a quarter wave plate and an analyzer. The interference signal contains information about the projection angle of the analyzer, which is hidden by the phase noises. The nonlocal correlations between the projection angles of two distant observers are established by analyzing their data through analog signal multiplication without any post-selection technique. This scheme can be used to implement Ekert's protocol for quantum key distribution. The implementation of two independent coherent states in this scheme is also discussed.

Quantum-entanglement aspects of polaron systems.

VLADIMIR STOJANOVIC, Carnegie Mellon University, MIHAJLO VANEVIC, University of Basel, Switzerland — We describe quantum entanglement inherent to the polaron ground states of coupled electron-phonon (or, more generally, particle–phonon) systems based on a model comprising both local (Holstein-type) and nonlocal (Peierls-type) coupling. We study this model using a variational method supplemented by the exact numerical diagonalization on a system of finite size. By way of subsequent numerical diagonalization of the reduced density matrix, we determine the particle-phonon entanglement as given by the von Neumann and linear entropies. Our results are strongly indicative of the intimate relationship between the particle localization/delocalization and the particle-phonon entanglement. In particular, we find a compelling evidence for the existence of a non-analyticity in the entanglement entropies with respect to the Peierls-coupling strength. The occurrence of such non-analyticity — not accompanied by an actual quantum phase transition — reinforces analogous conclusion drawn in several recent studies of entanglement in the realm of quantum-dissipative systems. In addition, we demonstrate that the entanglement entropies saturate inside the self-trapped region where the small-polaron states are nearly maximally mixed.

Entanglement generation under continuous parity measurement.

ANDREW JORDAN, Unv. of Rochester — We examine the stochastic dynamics of entanglement for an uncoupled two-qubit system, undergoing continuous parity measurement. Starting with a fully mixed state, the entanglement is zero for a finite amount of time, when it is suddenly created, which we refer to as entanglement genesis. There can be further entanglement sudden death/birth events culminating in the formation of a fully entangled state. We present numerical investigations of this effect together with statistics of the entanglement genesis time in the weak measurement limit as well as the quantum Zeno limit. An analytic treatment of the physics is presented, aided by the derivation of a simple concurrence equation for Bell basis X-states. The probability of entanglement border crossing and mean first passage times are calculated for the case of measurement dynamics alone. We find that states with almost the same probability of entanglement border crossing can have very different average crossing times. Our results provide insights on the optimization of entanglement generation by measurement.

Interferometric Determination of Concurrence of Unknown Two-Qubit Entanglement.

S.-S. B. LEE, H.-S. SIM, KAIST — We propose a scheme for both distilling and quantifying entanglement, applicable to individual copies of an arbitrary unknown two-qubit state. It is realized in a usual two-qubit interferometry with local filtering. Proper filtering operation for the maximal distillation of the state is achieved, by erasing single-qubit interference, and then the concurrence of the state is determined directly from the visibilities of two-qubit interference. For some representative quantum states, the efficiency is compared between our interferometric scheme and the full state tomography.

Scattering approach to the entanglement entropy area law for fermions.

GREGORY LEVINE, Hofstra University — The entanglement entropy (EE) of a critical fermion system coupled to another system by a “weak link” is studied. In this model, EE arises from two-qubit interference. For some representative quantum states, the efficiency is compared between our interferometric scheme and the full state tomography.

Mutual information and compactification radius in 3-qubit GHZ-class states.

SHOHINI GHOSE, NEIL SINCLAIR, SHANTANU DEBNATH, Wilfrid Laurier University. RENE STOCK, University of Toronto. PRANAW RUNGTA, IIS, India — Multiqubit entanglement is a crucial ingredient for large-scale quantum information processing, and has been the focus of several recent studies. Entanglement between qubits can lead to violations of Bell-type inequalities that are satisfied by local hidden variable models, indicating the nonlocal nature of the correlations between qubits. For 2-qubit pure states, bipartite entanglement is simply related to the Bell-CHSH nonlocality parameter. No such analytical relation between multipartite entanglement and nonlocality has yet been obtained for systems of three or more qubits. We have derived relationships between genuine tripartite entanglement and nonlocality for families of 3-qubit GHZ-class pure states. We quantify tripartite entanglement by the 3-tangle and derive its relationship to the Svetlichny inequality for testing tripartite nonlocality. For the class of generalized GHZ states, although the 3-tangle is always non-zero, we identify some states that do not violate the Svetlichny inequality. Furthermore, we show that states known as the maximal slice states always violate the Svetlichny inequality and analogous to the 2-qubit case, the amount of violation increases with the 3-tangle. The generalized GHZ states and the maximal slice states have unique tripartite entanglement and nonlocality properties in the set of all pure states.

Quantum Noise as an Entanglement Entropy Meter.

ISRAEL KLICH, University of Virginia, LEONID LEVITOV, MIT — Entanglement entropy, which is a measure of quantum correlations between separate parts of many-body systems, is defined solely in terms of the many-body density matrix, with no relation to any particular observables. Because of that, it has not been clear how to access this quantity experimentally. Here we unveil a universal relation between entanglement entropy of fermions and statistics of current flowing through a quantum point contact. This relation provides a way to experimentally measure entanglement entropy, and test seminal results of conformal field theory such as the prediction of Holzhey, Larsen and Wilczek for entanglement entropy, and test seminal results of conformal field theory such as the prediction of Holzhey, Larsen and Wilczek for entanglement entropy.
1:03PM J15.00010 Universal behavior of the entanglement entropy in 2D conformal quantum critical points and generalized quantum dimer models, BENJAMIN HSU, University of Illinois, Urbana-Champaign, MICHAEL MULLIGAN, Stanford University, EDUARDO FRADKIN, University of Illinois, Urbana-Champaign, EUN-AH KIM, Cornell University — We study the scaling behavior of the entanglement entropy of two dimensional conformal quantum critical systems, i.e., systems with scale invariant wave functions. They include two-dimensional generalized quantum dimer models on bipartite lattices and quantum loop models, as well as the quantum Lifshitz model and related gauge theories. We show that, under quite general conditions, the entanglement entropy of a large and simply connected sub-system of an infinite system has a universal contribution which is independent of the size of the region. This universal contribution is computable in terms of the properties of the underlying large-scale conformal structure of the wave function of these quantum critical systems.

1:15PM J15.00011 Theory of finite-entanglement scaling at one-dimensional quantum critical points, FRANK POLLMANN, SUBROTO MUKEERJEE, ARI TURNER, JOEL MOORE, UC Berkeley — We present a quantitative scaling theory of finite-entanglement approximations at one-dimensional quantum critical points. Finite-entanglement scaling is governed not by the scaling dimension of an operator but by the “central charge” of the critical point, which counts its universal degrees of freedom. An important ingredient is the universal distribution of density-matrix eigenvalues (the “entanglement spectrum”) at a critical point recently obtained by Calabrese and Lefevre. The theory is compared to the numerical error scaling of several quantum critical points, obtained by the infinite Time Evolved Block Decimation (iTEBD) method that extends the conventional Density-Matrix Renormalization Group (DMRG) algorithm.

1:27PM J15.00012 ABSTRACT WITHDRAWN

1:39PM J15.00013 Entanglement witnesses for n-qubit systems, RICHARD BONDE, ANDREW SCHAF, ELIZABETH BEHRMAN, Department of Physics, Wichita State University — We consider the entanglement of states under the renormalization-group (RG) transformations and apply it to the ground states of Hamiltonians that possess quantum phase transitions. We find that near critical points, the ground-state entanglement under RG transformation exhibits singular behavior. The singular behavior under finite steps of RG reveals the correlation length exponent. However, under the infinite steps of RG transformation, the singular behavior is rendered different, and it is not universal unless the critical point can be described by a conformal field theory.

1:51PM J15.00014 Comparisons of entanglement witnesses for n-qubit systems, RICHARD BONDE, ANDREW SCHAF, ELIZABETH BEHRMAN, Department of Physics, Wichita State University — An overlooked problem in witness design is the possibility of phase offset contamination. For example, the singlet EPS 2-qubit state $\frac{1}{\sqrt{2}} (|↑↓⟩ - |↓↑⟩)$ differs from $\frac{1}{\sqrt{2}} (|↑⟩|↓⟩ + |↓⟩|↑⟩)$ only by a relative phase factor of $e^{iπ}$, yet both states are fully entangled. We compare in detail several published witnesses on entangled pure and mixed systems with varying degrees of phase offset.

2:03PM J15.00015 ABSTRACT WITHDRAWN

Tuesday, March 17, 2009 11:15AM - 1:03PM — Session J16 DAMOP: Focus Session: Disorder in Ultra-Cold Gases 317

11:15AM J16.00001 The Role of Interactions in Disorder Induced Damping of Dipole Oscillations of a Bose-Einstein Condensate, SCOTT POLLACK, D. DRIES, T.A. CORCOVILOS, R.G. HULET, Rice Quantum Institute and Department of Physics and Astronomy, Rice University, Houston, TX 77005 — We investigate the damping of dipole oscillations of a $^7\text{Li}$ Bose-Einstein condensate (BEC) in a disordered optical potential. In our highly tunable system we vary the disorder strength $V_D$, the initial velocity of the BEC, and the chemical potential $\mu$ by adjusting the $s$-wave scattering length $a$ via a Feshbach resonance. We observe the breaking of superfluid flow, for values of $V_D$, as small as 0.1$\mu$, and cessation of motion for $V_D \sim \mu$. Counter-intuitively, at supersonic velocities the flow becomes asymptotically dissipationless regardless of the disorder strength. We test the validity of the scaling $V_D/\mu$ over several decades of $a$, including values of $a$ as small as 0.01$\mu$, where magnetic dipole effects dominate. We also report on observations of dissipative flow of nearly non-interacting ideal quantum gases and bright matter-wave solitons.

1Work supported by NSF, ONR, the Keck Foundation and the Welch Foundation.

11:27AM J16.00002 Disorder effects in the evolution from BCS to BEC superfluidity, LI HAN, CARLOS A. R. SA DE MELO, Georgia Institute of Technology — We discuss the effects of disorder on the critical temperature of superfluids during the evolution from BCS to BEC. For $s$-wave superfluids we find that the critical temperature is weakly affected by disorder in the BCS regime as described in Anderson's theorem, even less affected by disorder at zero chemical potential (near unitarity), but strongly affected by disorder in the BEC regime, where Anderson's theorem does not apply. This suggests that the superfluid is more robust to the effects of disorder at the interaction parameter where the chemical potential vanishes (close to unitarity). We construct a three dimensional phase diagram of critical temperature, disorder and interaction parameter $\lambda$, and show that there are regions of localized superfluidity, as well as insulating regions due to Anderson localization of fermions (BCS regime) and molecular bosons (BEC regime). The phase diagram for higher angular momentum (e.g. $p$-wave and $d$-wave) is also analyzed, where the effects of disorder are much more dramatic in the BCS regime in comparison to the $s$-wave case because pair breaking is strong, while the disorder effects in BEC regime are similar to what occurs in the $s$-wave case.

[1] Li Han, C. A. R. Sa de Melo, arXiv:0812.xxxx

We thank NSF (DMR-0709584) for support.
11:39 AM J16.00003 Magnetism Localization and Hole Localization in Fermionic Atoms Loaded on Optical Lattice, MASAHIKO OKUMURA, SUSUMU YAMADA, CCSE, Japan Atomic Energy Agency, NOBUHIKO TANIGUCHI, Institute of Physics, University of Tsukuba, MASAHIKO MACHIDA, CCSE, Japan Atomic Energy Agency — In order to study an interplay of disorder, correlation, and spin imbalance on antiferromagnetism, we systematically explore the ground state of one-dimensional spin-imbalanced Fermionic atoms loaded on an optical lattice by using the density-matrix renormalization group method [1]. We find that disorders localize the antiferromagnetic spin density wave induced by imbalanced fermions and the increase of the disorder magnitude shrinks the areas of the localized antiferromagnetized regions. Moreover, the antiferromagnetism finally disappears above a large disorder. We also study hole doped cases [2]. Concentrating on the doped-hole density profile, we find in a large U/\tau regime that the clean system exhibits a simple fluid-like behavior whereas finite disorders create locally Mott regions which expand their area with increasing the disorder strength contrary to the conventional sense. References [1] M. Okumura, S. Yamada, N. Taniguchi, and M. Machida, arXiv:0810.3953. [2] M. Okumura, S. Yamada, N. Taniguchi, and M. Machida, Phys. Rev. Lett. 101 016407 (2008).

12:03PM J16.00005 Dynamical Effects of Disorder in Optical Lattices, M. BEELER, E.E. EDWARDS, TAO HONG, S.L. ROLSTON, Joint Quantum Institute and Department of Physics, University of Maryland, National Institute of Standards and Technology — The precise control available in systems of neutral atoms confined in optical lattices makes them an ideal place to investigate the effects of disorder on crystal structure. We experimentally investigate how disorder affects the dynamical properties of these systems. Using a 1D optical lattice with the addition of one or two weak incommensurate traps, we investigate the adiabaticity criteria for loading the ground state of the disordered lattice. We find that even a very small amount of disorder greatly increases the timescale needed for adiabatic loading. We attribute this change to the large change in the ground state of the wavefunction with the addition of an impurity, as the wavefunction becomes localized. In addition, we will report on experimental efforts to study the effects of disorder in two-dimensional systems and on the timescales of thermalization in one dimension.

12:15PM J16.00006 Impurity crystal in a Bose-Einstein condensate, DAVID ROBERTS, Los Alamos National Laboratory, SERGIO RICA, Ecole Normale Superieure — We investigate the behavior of impurity fields immersed in a larger condensate field. The conditions for stability and collapse of this system will be presented. We discuss the localization of a single impurity field within a condensate and note the effects of surface energy. We derive the functional form of the attractive interaction between two impurities due to mediation from the condensate in 1, 2, and 3 dimensions. Generalizing the analysis to N impurity fields, we show that within various parameter regimes a crystal of impurity fields can form spontaneously in the condensate. Finally, we show the system of condensate and crystallized impurity structure to have nonclassical rotational inertia, which is characteristic of superfluidity, i.e. the system can be seen to exhibit supersolid behavior.

12:27PM J16.00007 Experiments on Disordered Quantum Gases, BRIAN DEMARCO, Univ of Illinois - Urbana — No abstract available.

Tuesday, March 17, 2009 11:15AM - 2:15PM — Session J17 GQI: Focus Session: Superconducting Phase Qubits

11:15AM J17.00001 High-fidelity gates in Josephson phase qubits, ERIK LUCERO, University of California, Santa Barbara — Complex algorithms for a quantum computer require error correction and robust calibration protocols for extended pulse sequences. We present significant progress towards both of these goals with our detailed measurements of gate fidelity and coupled qubit experiments with multi-pulse sequences. We measure single qubit gate fidelities of 0.98, limited by energy relaxation; and by carefully separating out gate and measurement error we construct a complete error budget. Using the new metrological technique of “Ramsey filtering” we show how one important error process can be measured and reduced to a level of 10^-4, a magnitude believed to be near the fault tolerant threshold. This measurement demonstrates that our quantum system remains in the two-state qubit manifold during our single qubit operations. This precision and accuracy is made possible by custom control electronics that can create arbitrarily shaped microwave pulses.

11:51AM J17.00002 Universal Quantum Gates in Josephson Junction Phase Qubits, RADOSLAW BIALCZAK, M. ANISMAN, M. HOFHEINZ, E. LUCERO, M. NEELEY, A. O’CONNELL, D. SANK, U.C. Santa Barbara, M. STEFFEN, IBM T.J. Watson Research Center, H. WANG, J. WENNER, A. CLELAND, J. MARTINIS, U.C. Santa Barbara — Josephson junction phase qubits are at a point where they can be used to create more complex operations such as quantum gates. Here we present work where we have tuned capacitively coupled Josephson junction phase qubits on and off resonance to generate and characterize a SQiSW gate using quantum process tomography (QPT). The SQiSW is the most fundamental universal gate for our system because it arises directly from the Hamiltonian for the physical circuit of our coupled qubits. In order to create more complex gates such as the CNOT, the SQiSW gate must be used to generate the entanglement. We perform QPT and obtain the Chi matrix, from which quantitative measures such as the gate fidelities can be calculated. We also show how to correct for measurement crosstalk and reduced visibilities present in our system and we perform measurements that quantitatively characterize the on/off ratio of our coupling scheme.

12:03PM J17.00003 Engineering Tripartite Entangled States of Two Phase Qubits Coupled via a Cavity, JAE PARK, FABIO ALTOMARE, RAY SIMMONDS, NIST — We present an experimentally inexpensive scheme for preparing certain tripartite entangled states. We suggest ways to test the degree to which such target states have been successfully prepared. We present a convenient geometrical interpretation of the resonant unitary dynamics which gives a natural interpretation for the characteristic frequencies and provides intuition for the pulse sequence necessary to achieve a desired target state.
12:15PM J17.00004 Two Qubits and a Cavity: Three’s Company. FABIO ALTOMARE, MICHAEL ALLMAN, KATARINA CICAK, JAE A. PARK, MIKA A. SILLANPAÄ, ADAM SIROIS, JOSHUA STRONG, JED WHITTAKER, RAYMOND W. SIMMONDS, National Institute of Standards and Technology, Boulder, CO (USA) — Quantum information theory suggests that there are two inequivalent classes of tripartite entanglement under stochastic local operations and classical communications (PRA, 62, 062314). Representative of these classes are the GHZ state and the W states, respectively. In this talk I will describe our experimental results on two superconducting phase qubits coupled through a cavity: one of the few cases where three is company and not a crowd. This system, effectively three coupled qubits if we restrict the cavity excitation to the single photon manifold, has allowed us to observe the spectroscopic signature and dynamics of Tripartite Entanglement. The rich dynamics of this system has allowed us to also observe a) Bell state between two qubits (with the third one disentangled), and b) W state between the three qubits. Future possibilities include the observation of GHZ state, particularly interesting for its practical applications, and for testing the non-locality of quantum mechanics.

1 Helsinki University of Technology

12:27PM J17.00005 Relaxation Dynamics of Fock States in a High Q Microwave Resonator Coupled to a Superconducting Phase Qubit. HAOHUA WANG, MAX HOFHEIZN, MARKUS ANSMANN, RADOSLAW BIALCZAK, ERIK LUCERO, MATTHEW NEELEY, AARON O’CONNELL, DANIEL SANK, JIM WENNER, ANDREW CLELAND, JOHN MARTINIS, Department of Physics, University of California, Santa Barbara — We have improved the lifetime of our high Q microwave resonator that is coupled to a superconducting phase qubit. Using high speed electronics, we have successfully generated Fock states with up to 15 photons. We analyze the resonator number state using the qubit to verify the high purity of the Fock states. Finally we monitor the subsequent decay of the Fock states in time, and show that the decay matches that expected from theory, with the $n$-photon lifetime scaling as $T_1/n$, where $T_1$ is the one-photon lifetime. Measurements on the decay of the coherent states, generated in the resonator using classical pulses, are also in agreement with theory.

12:39PM J17.00006 Controllable Coherent Population Transfers in Superconducting Qubits for Quantum Computing. L.F. WEI, RIKEN and Southwest Jiaotong University, Chengdu 610031, China, J.R. JOHANSSON, L.X. CEN, S. ASHHAB, F. NORI — We propose an approach to coherently transfer populations between selected quantum states in one- and two-qubit systems by using controllable Stark-chirped rapid adiabatic passages. These evolution-time insensitive transfers, assisted by easily implementable single-qubit phase-shift operations, could serve as elementary logic gates for quantum computing. Specifically, this proposal could be conveniently demonstrated with existing Josephson phase qubits. Our proposal can find an immediate application in the readout of these qubits. Indeed, the broken parity symmetries of the bound states in these artificial atoms provide an efficient approach to design the required adiabatic pulses.

12:51PM J17.00007 Three and Four Coupled Josephson Junction Phase Quubits. ZECHARIAH THRAILKILL, JOSEPH LAMBERT, SAM KENNERLY, ROBERTO RAMOS, Drexel University — The Josephson junction phase qubit has been shown to be a viable candidate for quantum computing. The two coupled phase quibit system has been extensively studied theoretically and experimentally. We have analyzed the quantum behavior of systems with more, three and four capacitively-coupled phase quibits, with different possible configurations. We have used anharmonic oscillators to model the systems. We will discuss some of the properties of these simple networks. The focus is on natural state evolution using a time independent, or adiabatically changing Hamiltonian. Analyzing how to transfer quantum information from one qubit to another and performing operations to change the overall state of these systems will give a better understanding of how to utilize the different qubit configurations. We will report on the progress of spectroscopic measurements for the three phase quibit systems.

1:03PM J17.00008 Tunable Cavity QED with Josephson Phase Quibits. JOSHUA STRONG, NIST — We have designed a tunable Josephson resonator and have coupled it to two phase quibits. The resonator can act as a cavity for QED-type experiments. We discuss results.

1:15PM J17.00009 Emulation of spin dynamics using a superconducting phase qudit. MATTHEW NEELEY, M. ANSMANN, R. BIALCZAK, M. HOFHEIZN, E. LUCERO, A. O’CONNELL, D. SANK, H. WANG, J. WENNER, JOHN MARTINIS, ANDREW CLELAND, UC Santa Barbara — In superconducting quantum circuits, the nonlinearity of the Josephson junction allows energy-level transitions to be addressed individually by their unique frequencies. Typically this is used to operate the system as an effective two-level system, a qubit. In a recent experiment, we extended our coherent control of a phase qubit to the first five energy levels, allowing us to operate the device as a qudit with $d = 3$, $4$, or $5$. We use this system to emulate the dynamics of single spins with spin quantum number $s = 1/2$, $1$ and $3/2$. We show that the phase acquired by a spin under rotation around a closed path follows the theoretical prediction. In particular, we confirm the even (odd) parity of integer (half-integer) spins under $2\pi$ rotation.

1:27PM J17.00010 Multiplexed Phase qubit readout using SQUID-resonators. JED WHITTAKER, MICHAEL ALLMAN, University of Colorado at Boulder, FABIO ALTOMARE, KATARINA CICAK, DALE LI, JAE PAK, NIST, ADAM SIROIS, JOSHUA STRONG, University of Colorado at Boulder, RAYMOND SIMMONDS, NIST — Flux biased phase quibits have traditionally been read out using a critical current switching technique of a coupled DC SQUID. This method has three limitations: it is extremely slow (orders of magnitude longer than typical energy relaxation times), difficult to multiplex, and by exceeding the critical current, it is dissipative and feeds broadband radiation back into the qubit, decohering its state. We are developing a SQUID-resonator readout method that addresses all three of these limitations. By operating the SQUID as a resonator, we can measure the state of the quibit quickly (on the order of its coherence time), we can multiplex resonant readout lines, and we can operate on the SQUID’s supercurrent branch eliminating dissipation and decohering radiation. This faster, quieter readout should allow us to use measured results for real-time quantum feedback.

1:39PM J17.00011 Berry’s Phase of a Current-Biased Josephson Junction. ANTHONY TYLER, Drexel University, ROBERTO RAMOS, ZECHARIAH THRAILKILL, SAM KENNERLY, Drexel University — A quantum system, prepared in an eigenstate, can accumulate a geometric phase known as Berry’s phase in addition to the expected dynamic phase. This occurs when there are adiabatic changes to the Hamiltonian which trace a closed loop in parameter space. A common example of this phase is an electron in a slowly varying magnetic field which traces a closed path. From this adiabatic variation, the electron’s spin state has acquired a Berry’s phase in addition to the dynamic phase. Due to the similarities between spin-1/2 particles, such as the electron, and solid state quantum bits (qubits), there should be an analogous process by which these systems can gain a Berry’s phase. Such processes have been tested in the charge qubit and has been derived for the flux qubit. Here, we will derive the Berry’s phase for a phase qubit which can be found experimentally using quantum state tomography. We then utilize this to explore the possibility of creating topological gates with phase qubits.

1 Please address all correspondences to rcr32@drexel.edu
Nürnberg, Erwin-Rommel-Strasse, 1, D-91058 Erlangen, Germany — An intrinsic SQUID is a superconducting ring made of Bi, X.Y. JIN, J. LISENFELD, Y. KOVAL, A. LUKASHENKO, A.V. USTINOV, P. MÜLLER, Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse, 1, D-91058 Erlangen, Germany — An intrinsic SQUID is a superconducting ring made of Bi-Sr2CaCu2O8, δ single crystal, intercepted by two intrinsic Josephson junction stacks. The inductance parameter βL can be tuned in a wide range by changing the height and the cross-section area of the stacks. When biased with dc current, the device showed typical properties of hysteretic dc-SQUIDs. When a device was coupled with a coil and a Nb readout dc-SQUID, typical rf-SQUID behavior was observed. By choosing a proper reset field, quantum escape from a single minimum has been measured on a sample of βL ≈ 10. The escape rate can be fine-tuned by applying short pulses down to 1 ns, which allows a fast readout technique. With these prerequisites achieved, our experiments have opened the path to directly using these intrinsic SQUIDs as high-Tc phase qubits. The first attempts to measure Rabi oscillations on these devices will be discussed.

2:03PM J17.00013 GHZ protocols for superconducting qubits1. ANDREI GALIAUTDINOV, University of Georgia, JOHN MARTINS, U. C. Santa Barbara — Superconducting circuits with Josephson junctions gained considerable attention as promising candidates for scalable solid state quantum computing architectures. While macroscopic quantum behavior of such circuits has already been demonstrated (e.g., Rabi oscillations, high fidelity state preparation and measurement, various logic gate operations, etc.), further progress in developing a workable quantum computer will depend crucially on architecture’s ability to implement various multibit entangled states. Here we show how Greenberger-Horne-Zeilinger states can be generated in tripartite systems with capacitive and inductive couplings. Generalization to architectures containing arbitrary numbers of qubits is also discussed.

Tuesday, March 17, 2009 11:15AM - 2:15PM — Session J18 DMP DPOLY: Charge Transport and Optical Properties of Organic Semiconductors

11:15AM J18.00001 Light Emitting Transistors of Organic Single Crystals, YOSHIHIRO IWASA, Tohoku University — Organic light emitting transistors (OLETs) are attracting considerable interest as a novel function of organic field effect transistors (OFETs). Besides a smallest integration of light source and current switching devices, OLETs offer a new opportunity in the fundamental research on organic light emitting devices. The OLET device structure allows us to use organic single crystals, in contrast to the organic light emitting diodes (OLEDs), the research of which have been conducted predominantly on polycrystalline or amorphous thin films. In the case of OFETs, use of single crystals have produced a significant amount of benefits in the studies of pursuit for the highest performance limit of FETs, intrinsic transport mechanism in organic semiconductors, and application of the single crystal transistors. The study on OLETs have been made predominantly on polycrystalline films or multicomponent heterojunctions, and single crystal study is still limited to tetracene [1] and rubrene [2], which are materials with relatively high mobility, but with low photoluminescence efficiency. In this paper, we report fabrication of single crystal OLETs of several kinds of highly luminescent molecules, emitting colorful light, ranging from blue to red. Our strategy is single crystallization of monomer or oligomeric molecules, which are known to have a very high photoluminescence efficiency. Here we report the result on single crystal LETs of rubrene (red), 4,4'-bis(diphenylyvinyleyl)-anthracene (green), 1,4-bis(5-phenylthiophene-2-yl)benzene (AC5) (green), and 1,3,6,8-tetraphenylpyrene (TPPy) (blue), all of which displayed ambipolar transport well as well as peculiar movement of voltage controlled movement of recombination zone, not only from the surface of the crystal but also from the edges of the crystals, indicating light confinement inside the crystal. Realization of ambipolar OLET with variety of single crystals indicates that the fabrication method is quite versatile to various light emitting molecular solids, providing novel opportunities to get further insight on the intrinsic optoelectronic processes in organic semiconductors.


11:51AM J18.00002 ABSTRACT WITHDRAWN —

12:27PM J18.00003 Modification of the electronic properties of rubrene crystals by extrinsic species, LEONIDAS TSETSERIS, Vanderbilt University and University of Thessaloniki (Greece), SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The chemical stability of organic semiconductors is one of the most important factors for the performance of related electronic devices. Here, we report the results of first-principles calculations on the effect of some of the most typical defect culprits in the prototype system of rubrene, the current record-holder organic semiconductor in terms of carrier mobilities. We identify the most stable water and oxygen-related impurity structures, with opportunities for nanoscale surface functionalization of organic semiconductors and provides experimental access to the regime of high carrier density. Here, we report the results of first-principles calculations on the effect of some of the most typical defect culprits in the prototype system of rubrene, the current record-holder organic semiconductor in terms of carrier mobilities. We identify the most stable water and oxygen-related impurity structures, with opportunities for nanoscale surface functionalization of organic semiconductors and provides experimental access to the regime of high carrier density. Here, we report the results of first-principles calculations on the effect of some of the most typical defect culprits in the prototype system of rubrene, the current record-holder organic semiconductor in terms of carrier mobilities. We identify the most stable water and oxygen-related impurity structures, with opportunities for nanoscale surface functionalization of organic semiconductors and provides experimental access to the regime of high carrier density.

12:39PM J18.00004 Charge carrier transport and optical properties of SAM-induced conducting channel in organic semiconductors, VITALY PODZOROV, Rutgers University — Certain types of self-assembled monolayers (SAM) grown directly at the surface of organic molecular crystals can induce a high surface conductivity in these materials [1]. For example, the conductivity induced by perfluorinated alkyl silanes in organic molecular crystals approaches 10 to -5 Siemens per square. The observed large electronic effect opens new opportunities for nanoscale surface functionalization of organic semiconductors and provides experimental access to the regime of high carrier density. Here, we discuss the results of an extensive study of SAM-induced conductivity in several types of organic semiconductors. [1] M. F. Calhoun, J. Sanchez, D. Olaya, M. E. Gershenson and V. Podzorov, “Electronic functionalization of the surface of organic semiconductors with self-assembled monolayers”, Nature Mat. 7, 84 (2008).

12:51PM J18.00005 Infrared spectroscopy of organic semiconductor modified by self-assembled monolayers, O. KHATIB, University of California, San Diego, B. LEE, V. PODZOROV, Rutgers University, J. YUEN, A.J. HEEGER, University of California, Santa Barbara, Z.Q. LI, M. DI VENTRA, D.N. BASOV, University of California, San Diego — Recently, self-assembled monolayers (SAMs) were used to modify electronic surface properties of organic single crystals, leading to several orders of magnitude increase in the electrical conductivity. Motivated by this discovery, the same technique was applied to polymers. Here we present a thorough spectroscopic investigation of organic semiconductors based on poly(3-hexithiophene) (P3HT) that have been treated with a fluorinated trichlorosilane SAM. Infrared spectroscopy offers access to details of charge injection, electrostatic doping, and the electronic structure that are not always available from transport measurements, which can be dominated by defects and contact effects in organic films. The SAM molecules penetrate into the bulk, leading to a rich spectrum of electronic excitations in the mid-infrared energy range. [1] M. F. Calhoun, J. Sanchez, D. Olaya, M. E. Gershenson, V. Podzorov, “Electronic functionalization of the surface of organic semiconductors with self-assembled monolayers”, Nature Mater. 7, 84–89 (2008).
grain size is 29 of FTES-ADT; varying the FTES-ADT concentration by 2-fold induces a 3-order of magnitude change in the grain size. For channels in which the average can seed the crystallization of TES-ADT during solvent-vapor annealing. The grain size in these films follows an exponential dependence on the concentration phene (TES-ADT) films through the addition of fractional amounts of fluorinated 5,11-bis(triethylsilylethynyl) anthradithiophene (FTES-ADT). FTES-ADT YUEH-LIN (LYNN) LOO, Princeton University — We present a novel method for controlling the grain size in solution-processed triethylsilylethynyl anthradithiophene (TES-ADT) films through the addition of fractional amounts of fluorinated 5,11-bis(triethylsilylethynyl) anthradithiophene (FTES-ADT). FTES-ADT can seed the crystallization of TES-ADT during solvent-vapor annealing. The grain size in these films follows an exponential dependence on the concentration of FTES-ADT; varying the FTES-ADT concentration by 2-fold induces a 3-order of magnitude change in the grain size. For channels in which the average grain size is 29 μm, device mobility of the organic thin-film transistors (OTFTs) is 0.05 cm²/V·s. For channels in which the average grain size is 2700 μm, the device mobility is 0.35 cm²/V·s. The relationship between device mobility and grain size is well described by a composite mobility model, which assumes a high intrinsic grain mobility and a low grain boundary mobility. Grazing incidence x-ray diffraction indicates that the crystal lattice of TES-ADT is preserved despite the addition of FTES-ADT:


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2:03PM J18.00011 Low temperature, field-dependent mobility in pentacene thin-film transistors. ADRIAN SOUTHERD, Center for Nanophysics and Advanced Materials (CNAM) and the Department of Physics (DOP), University of Maryland (UM), VINOD SANGWAN, Laboratory of Physical Sciences (LPS), CNAM, and DOP, UM, DAN LESKNI, MICHAEL FUHRER, CNAM and the DOP, UM, ELLEN WILLIAMS, LPS, CNAM, and the DOP, UM — We measure the field-effect and saturation mobility of Au bottom contact thin-film polycrystalline pentacene field-effect transistors while varying temperature, channel length, and gate voltage. We utilize Au bottom contacts without a wetting layer, and achieve contact resistance as low as 1 kΩ·cm despite disturbance of the pentacene morphology at the drain and source electrodes. By measuring multiple channel lengths, we extract a contact-resistance free mobility. We confirm this value using an alternative technique in which we short the source and drain electrodes and make two terminal measurements of the capacitance and loss between these electrodes and the gate as a function of frequency. We discuss the result of the mobility in the context of Poole-Frenkel theory to rationalize the non-linear dependence of drain current on drain voltage, and test the predictions of recently developed models for transport in such systems.

Supported by the Laboratory for Physical Science at UM.

Tuesday, March 17, 2009 11:15AM - 2:15PM -
Session J19 DPOLY: Block Copolymer Thin Films II
11:15AM J19.00001 Self-assembled surface patterns from organometallic-containing triblock terpolymers , VIVIAN CHUANG, CAROLINE ROSS, Massachusetts Institute of Technology, JESSICA GWYThER, IAN MANNERS, University of Bristol — Block copolymers are useful in nanotechnology because they can self-assemble to form periodic nanostructures. Here, we demonstrate the formation of hollow ring arrays with a period of 54 nm from a core-shell cylindrical-morphology poly(styrene-b-ferrocenylmethylsilane-b-2-vinyl pyridine) (PS-b-PFS-b-P2VP) triblock terpolymer thin film. By spin-coating and solvent annealing, thin films of the polymer were self-assembled into arrays of core-shell structures oriented perpendicular to the top surface of the film. Various chemically modified substrates were employed to investigate the effects of interfacial interaction between the substrate and the film, as well as the effects of solvent annealing, on the film morphology. Results will be compared with those obtained from a poly(butadiene-b-styrene-b-methyl methacrylate) triblock terpolymer [1]. The PS core and P2VP matrix blocks were partly removed simultaneously using oxygen plasma, and the remaining PFS ring pattern was successfully transferred into a PS layer by imprinting.


11:27AM J19.00002 Improvement of Extraction Efficiency of LED with Surface Relief Nanostucture Fabricated by Self-Assembled Block Copolymer Pattern , RYOTA KITAGAWA, AKIRA FUJIMOTO, KOJI ASAKAWA, Corporate Research & Development Center, Toshiba Corporation — A surface relief nanostructure was fabricated on the emission surface of light-emitting diodes (LEDs) using a self-assembled diblock copolymer pattern. The pattern of the nanostructure possesses moderate short-range order with slightly deviation in size and spacing, which is different from conventional extraction surface structures, such as photonic crystal and randomly textured surface. The dot pattern of a self-assembled polystyrene -polymethylmethacrylate diblock copolymer (PS-b-PMMMA) was used as an etched mask. An average dot spacing was controlled by changing blend ratio of PS-b-PMMMA, homo (h-) PS, and h-PMMMA in a polymer solution. In the photoluminescence (PL) measurement, the light extraction efficiency of the nanostructure exceeded over twice, compared with a flat surface, by optimizing the average spacing of the nanostructure. It was also revealed that the nanostructure showed more than 10% higher extraction efficiency than the highly ordered nanostructure fabricated by a self-assembled nanosphere pattern. These results can be interpreted as a contribution of structural fluctuation in the nanostructure for enhancement of extraction efficiency.

11:39AM J19.00003 Self-Assembling Block Copolymer Resist Mixtures toward Lithographic Resists for Sub-10 nm Features , CURRAN CHANDLER, VIKRAM DAVA, JAMES WATKINS, University of Massachusetts Amherst — Significant improvements in 193 nm photolithography have enabled the extension of device feature sizes beyond the 45 nm and 32 nm nodes, yet uncertainty lies beyond 22 nm features as no single replacement has emerged. Here we show that low molecular weight, nonionic block copolymer surfactant blends are capable of self-assembling into highly ordered domains with feature sizes on the order of 5 nm. These surfactants, most of which lack the required $\chi N$ for microphase separation on their own, exhibit strong segregation and long-range order upon addition of a component capable of multi-point hydrogen bonding that is specific for one of the blocks in the copolymer. This has been demonstrated by our SAXS study for self-assembled (PS-b-PPO-b-PEO) and Brij (PEO-4-(CH$_2$)$_3$CH$_3$) surfactants of various molecular weights and PEO volume fractions. Furthermore, we employ these highly-ordered systems as thin film, nanolithographic etch masks for the transfer of 10 nm patterns into silicon-based substrates. Small molecule, hydrogen bonding additives containing aromatic or silsesquioxane structure are also used to tune etch contrast between the blocks which is important for reducing line edge roughness (LER) of such small features.

11:51AM J19.00004 Directed assembly of block copolymers on chemically nanopatterned substrates: enabling science for ultra high resolution lithography , PAUL NEALEY, University of Wisconsin — Self-assembling materials based on block copolymers spontaneously form structures with well-defined dimensions and shapes at length scales of interest in nanotechnology. Unfortunately the thermodynamic driving forces for self-assembly are small and low-energy defects can get easily trapped. At issue is the extent of direction or guidance required to meet criteria related to perfection and registration for use of such materials in nanofabrication. Through fundamental understanding of the physics, chemistry, and surface and interfacial phenomena associated with equilibrating block copolymer films in the presence of chemically nanopatterned substrates, we demonstrate how block copolymers may be integrated into and advance the performance of the lithographic process. The technological importance of this approach is discussed with respect to patterned media and the fabrication of integrated circuits.

12:03PM J19.00005 Conditions for the directed assembly of thick block copolymer films on chemically nano-patterned surfaces , ADAM M. WELANDER, PAUL F. NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin, Madison, WI 53706 — The extent to which a lamellae forming block copolymer (bulk period, $L_0 = 48$ nm) can be directed to assemble on chemically nano-patterned striped surfaces (period $L_S$) with domains registered to and extending vertically away from the underlying pattern with few defects was studied as a function of film thickness, commensurability between $L_S$ and $L_0$, and temperature. The thickness through which low defect assembly could be achieved increased as $L_S$ and $L_0$ became more commensurate and as the temperature increased from 190 °C to 230 °C. Under certain conditions ($L_S \approx L_0 \approx 230$ °C), block copolymer films approaching 750 nm (aspect ratio $\approx 30$) in thickness still exhibited low levels of defectivity. These results were interpreted in terms of a phenomenological model and minimization of free energy including surface and interfacial energies and chain configuration entropy.

12:15PM J19.00006 Directed self-assembly of diblock copolymer thin films on chemically-patterned substrates for defect-free nano-patterning , MIKIHIITO TAKENAKA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, YASUHIKO TADA, Materials Research Laboratory, Hitachi Ltd., SATOSHI AKASAKA, SYNUKE ABURAYA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, HIROSHI YOSHIDA, Materials Research Laboratory, Hitachi Ltd., HIROKAZU HASEGAWA, Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, ELIZABETH DOBISZ, DAN KERCHER, San Jose Research Center, Hitachi Global Storage Technologies — We demonstrate that Polystyrene-block-poly(methyl methacrylate) (PS-b-PMMMA) can self-assemble in a well-aligned, long-range ordered nano-pattern over an area large enough to form micropatterned with chemically pre-patterned, templates prepared by electron beam (EB) lithography. We also demonstrate that the self-assembly process can interpolate points in between the EB generated pattern, thus multiplying the pattern density. Moreover, we show the results of the investigation about the time-evolution of the self-assembled structure during annealing process.

12:27PM J19.00007 Lamellar and Non-bulk like Morphologies in Thin Films of Block Copolymer on Chemical Nanopatterned Surfaces , GUOLIANG LIU, FRANCOIS DETCHEVEREY, JUAN J. DE PABLO, PAUL F. NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, 1415 Engineering Drive, Madison, WI, 53706 — Thin films of symmetric PS-b-PMMMA (bulk lamellae period $L_0$) were equilibrated on substrates patterned with periodic stripes such that the adjacent stripes are preferentially wet by the two blocks of the copolymer. The morphology of the films was quantified as a function of the following pattern characteristics: the period, $L_S$, where $L_S = \delta L_0$, $1 \leq \delta \leq 3$, the width of the PMMA wetting strips, $W$, and the interfacial energies between the blocks and the patterned stripes, $\chi_{i,j}$. Under different boundary conditions we can i) direct the assembly of lamellae perpendicular to the substrate and ordered in linear arrays so as to increase the density of features of the chemical pattern, or ii) obtain a number of stable non-bulk like structures including asymmetric lamellae, mixed orientated lamellae, dots, and check-board structures. The experimental results are compared to a phase-diagram predicted from molecular simulations.
Patterns Made from Electro-oxidation Nanolithography, JI XU, ANTONIO CHECCO, BENJAMIN OCKO, SOOJIN PARK, SHILIU WANG, THOMAS RUSSELL — The effect of confinement from chemical patterns on the self-assembly of block copolymer and related wetting physics has been studied. A variety of geometries designed in a mesh fashion were chemically patterned on OTS modified silicon wafers by electro-oxidation nanolithography. Thin films of a cylinder-forming PS-b-PEO were spin coated onto these patterned substrates. Thermal annealing of these films showed that the films were pinned on the patterned regions, due to the strong interaction between PEO block and carboxylic acid group on patterned surface while, over the non-patterned areas, dewetting was suppressed. The non-favorable interactions of both blocks with the substrate in the non-patterned areas caused the cylindrical microdomains to orient normal to the surface, being confined geometrically by the patterned regions. Defect-free, hexagonally packed cylindrical microdomains that conformed to hexagonal pattern written onto the surface were obtained. Point defects arose in the hexagonal packing of the microdomains when the dimensions or shape of the pattern were not commensurate with the natural packing of the copolymers.

12:51PM J19.00009 Time-Resolved SAXS Characterization of Block Copolymer Blends on Chemically Nanopatterned Surfaces, KARL STUEN, PAUL NEALEY, Univ. of Wisconsin-Madison Dept. of Chem. and Biol. Eng., DILLIP SATAPATHY, KIM NYGARD, HARUN SOLAK, Dept. of Synchrotron Rad. and Nanotech., Paul Scherrer Institut, Switzerland — The directed assembly of block copolymer/homopolymer ternary blend thin films on chemically nanopatterned substrates was investigated with in situ transmission SAXS. A ternary blend was used to match the block copolymer period with the period of a chemical pattern fabricated by x-ray interference lithography. The domain assembly in a 24-nm-thick block copolymer blend film on the chemical nanopattern was monitored with SAXS in real-time as a sample was heated from 100 to 240 °C at about 20 °C per minute. The strongest diffraction from the sample was detected after just 4.5 minutes of annealing (maximum temperature ~190 °C). Complementary results were obtained from top-down SEM images of films that were quenched to room temperature after various times during the temperature ramp. The SEM images revealed transient structures in the annealing process that may relate to the non-uniform distribution of homopolymer in the direction perpendicular to the substrate. The results were compared to previously reported Monte Carlo molecular simulations to better understand the three-dimensional structures that form during the annealing process.

1:03PM J19.00010 Imaging Layer Effect on Density Multiplication in the Directed Assembly of Block Copolymer Thin Films, HIUMAN KANG, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, EUNGNACK HAN, PADMA GOPALAN, Department of Materials Science and Engineering, University of Wisconsin-Madison, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — We report a new parallel patterning technique, molecular transfer printing (MTP), for replicating geometrically complex patterns over macroscopic areas with sub-15 nm feature dimensions, and the ability to replicate the same pattern multiple times. In MTP, inks are mixed with block copolymers (BCPs) and deposited as films on a substrate. The inks are compatible with only one block of the BCP, and separated into domains of nanometer scale dimensions after microphase separation. A second substrate is then placed in contact with the surface of the film. By designing the inks to react, adsorb, or otherwise interact with the second substrate, inks are transferred to the second substrate in the exact pattern of domains present at the surface of the “master” BCP film. Here we demonstrate high degrees of perfection on both line and dot patterns. We also show that 1) the master template can be regenerated, 2) the resultant replica can be used to direct the assembly of BCPs as a daughter master for MTP, and 3) the master and daughter templates can be reused tens of times.

1:15PM J19.00011 Molecular Transfer Printing Using Block Copolymers, SHENGXIANG JI, CHI-CHUN LIU, GUOLIANG LIU, PAUL NEALEY, Department of Chemical & Biological Engineering, University of Wisconsin-Madison — A molecular model of block copolymer systems is used to conduct a systematic study of the morphologies that arise when thin films of symmetric, lamellar forming block copolymer materials are deposited on nanopatterned surfaces. Over 500 distinct cases are considered. It is found that, in general, three distinct morphologies can arise depending on the strength of the substrate-polymer interactions, the film thickness, and the period of the substrate pattern. The relative stability of those morphologies is determined by direct calculation of the free energy differences. The dynamic propensity of those morphologies to emerge is examined by careful analysis of simulated trajectories. The results of this systematic study are used to interpret recent experimental data for films of polystyrene-PMMA copolymers on chemically nanopatterned surfaces.

1:27PM J19.00012 Pattern interpolation in thin films of lamellar, symmetric copolymers on nano-patterned substrates, FRANCOIS DETCHEVERRY, UMGANG NAGPAL, GUOLIANG LIU, PAUL NEALEY, JUAN DE PABLO, University of Wisconsin — A molecular model of block copolymer systems is used to conduct a systematic study of the morphologies that arise when thin films of symmetric, lamellar forming block copolymer materials are deposited on nanopatterned surfaces. Over 500 distinct cases are considered. It is found that, in general, three distinct morphologies can arise depending on the strength of the substrate-polymer interactions, the film thickness, and the period of the substrate pattern. The relative stability of those morphologies is determined by direct calculation of the free energy differences. The dynamic propensity of those morphologies to emerge is examined by careful analysis of simulated trajectories. The results of this systematic study are used to interpret recent experimental data for films of polystyrene-PMMA copolymers on chemically nanopatterned surfaces.

1:39PM J19.00013 Thin Films of Polydimethylsiloxane-Containing Block Copolymers, MAURICE WADLEY, KEVIN CAVICCHI, The University of Akron — The self-assembly of block copolymers into ordered nanostructures such as spheres, cylinders, and lamellae in the range of 10-100 nm makes them interesting materials for patterning surfaces. Thin films of poly(dimethylsiloxane) (PDMS) containing block copolymers are attractive for patterning due to their high oxygen etch resistance compared to other polymers. The main disadvantage of these polymers for patterning is the low surface tension of PDMS. This causes the preferential migration of PDMS to the air/film interface driving the formation of domains parallel to the surface and wetting layers. In this work a series of AB block copolymers containing PDMS have been prepared via RAFT polymerization where the surface tension of the opposing block was varied. Using a macro chain transfer approach, it is possible to isolate the effect of changing the opposing block while keeping the PDMS the same in each different block copolymer. The effect of changing the surface tension mismatch between the blocks on the thin film morphology will be discussed.

1:51PM J19.00014 Interfacial Bending of Lamellar Microdomains of Block Copolymers, SANG-MIN PARK, IBM Almaden Research Center, MENG DONG, Department of Chemical and Biological Engineering, Colorado State, CHARLES RETTNER, IBM Almaden Research Center, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State, HO-CHEOL KIM, IBM Almaden Research Center — We report our investigation on the interfacial bending property of the lamellar microdomains using a symmetric block copolymer of poly(styrene-b-methyl methacrylate) (PS-b-PMMA) deposited on a neutral surface. The degree of interfacial bending of lamellae on surface was controlled by varying the angle of elbow-like topographic guiding patterns prepared by E-beam lithography. The characteristic parameters of lamellae bending including the critical angles of elbow-like patterns which give maximum interfacial bending of lamellae, the lamellae tilting angle at sidewall were determined for both single and paired guiding patterns. The behavior of a block copolymer containing hybrid systems a minimum of poly(styrene-b-ethylene oxide) and organosilicate, was investigated as well. A computational calculation on the lamellae bending which provides more insights on the free energy and interfacial characteristics will be discussed as well.
2:03PM J19.00015 Observation of Surface Corrugation-Induced Alignment of Lamellar Microdomains in PS-b-PMMA Thin Films. HO-CHEOL KIM, SANG-MIN PARK, CHARLES RETTNER, IBM Almaden Research Center, BRIAN BERRY, Department of Chemistry, University of Arkansas at Little Rock, ELIZABETH DOBisz, Hitachi Global Storage Technologies

Previously we reported the alignment of lamellar microdomains of a block copolymer containing hybrid on a corrugated surface, which provides self-assembled crossbar nanostructures. The alignment of lamellae of the hybrid system is believed due to the anisotropic bending periphery of lamellae. Attempts to similarly align the lamellae of PS-b-PMMA using the same length scales of surface corrugation were not successful. In this study, we investigated the alignment of lamellar microdomains of PS-b-PMMA using even broader range of length scales of the surface corrugation. Within specific ranges of roughness scales, we observed that the lamellar microdomains of PS-b-PMMA align perpendicular to the direction of surface corrugation. The effect of relative scales of periodicity and film thickness of PS-b-PMMA to those of surface corrugation on the alignment of lamellae is discussed in this paper.

Tuesday, March 17, 2009 11:15AM - 1:27PM
Session J20 DPOLY: Frank J. Padden Jr. Award Symposium 321

11:15AM J20.00001 Pressure Effects on Polymer Coil-Globule Transitions near an LCST. DAVID SIMMONS, ISSAC SANCHEZ, University of Texas at Austin — A model for the pressure - temperature behavior of the coil-globule transition (CGT) of a polymer in dilute solution is developed without adjustable parameters. The predicted pressure-temperature conformational behavior semi-quantitatively correlates with extant experimental data. The model yields a heating induced coil-to-globule transition (HCGT) temperature that increases with pressure until it merges with a cooling induced coil-to-globule transition (CCGT). The point at which the CCGT and HCGT meet is a hypercritical point that also corresponds to a merging of lower critical solution temperature (LCST) and upper critical solution temperatures (UCST). Theoretical results are discussed in terms of a generalized polymer/solvent phase diagram that possesses two hypercritical points.

11:27AM J20.00002 Structure-property relationships in ABA copolymer gels with A homopolymer additions. MICHELLE SEITZ, Northwestern University, REBECCA ROTTSSLK, William Fremd High School, KIRT PAGE, NIST, KENNETH SHULL, Northwestern University — ABA acrylic triblock copolymers with poly(methyl methacrylate) endblocks and poly(butyl acrylate) midblocks transition from free flowing liquids to elastic solids with decreasing temperature in alcohol solvents. Homopolymer PMMA chains can be solubilized in the micelle cores if they are shorter than the endblocks. Indentation and compression tests were used to determine gel’s modulus and large strain behavior. Gels with volume fractions of PMMA less than ~0.2 are highly elastic and have modulus dictated by stretching of bridging midblocks. At higher PMMA contents, gels exhibit greater permanent deformation and moduli over an order of magnitude larger than would be expected from rubber elasticity alone. Small angle X-ray and neutron scattering and mean field simulations were used to correlate changes in gel structure and micelle morphology with the addition of homopolymer.

11:39AM J20.00003 A Versatile Method by Layer Assembly of Thin Organic Films. HERNAN R. RENGIFO, Columbia University, CRISTIAN GRIGORAS, University of Pennsylvania, JEFFREY KOBERSTEIN, Columbia University — Layer by layer (Lbl) assembly techniques construct multilayer thin films by sequential deposition of monomolecular layers of organic molecules. One of the drawbacks associated with their use is that monomolecular layers are usually held together by relatively weak forces such as Van der Waals, electrostatic and hydrogen bonding interactions, and can therefore be lacking in mechanical integrity. We demonstrate herein that heterofunctional polymers, functionalized with one azide chain terminus and a protected alkyne group as the other chain terminus, constitute a powerful and versatile means for the covalent layer-by-layer (Lbl) assembly of thin polymer films. Each monomolecular polymer layer is covalently bound to both the preceding and following layers to produce a robust multilayer structure. Because the coupling chemistry used, “click” chemistry, is highly chemoselective, the layering process is virtually independent of the chemical nature of the polymer so that the constitution of each layer can be selected at will.

1 Columbia University Center of Excellence in Genomic Science under NIH award P50 HG002806, DMR-0703054 from the National Science Foundation.

11:51AM J20.00004 How do entangled polymeric liquids flow? SHAM SUNDAR RAVINDRANATH, SHI-QING WANG, University of Akron — This work focused on investigating fundamental questions in polymer dynamics such as how entangled polymeric liquids respond to fast external deformation. By developing an effective particle tracking velocimetric (PTV) method, along with conventional rheometric measurements, new insights can be gained into the phenomenology of entangled polymers in presence of startup shear, step strain and large amplitude oscillatory shear (LAOS). During startup shear of well entangled systems, the shear field becomes inhomogeneous after the stress overshoot for a range of applied shear rates beyond the Newtonian region [1]. The emergence of shear banding after stress overshoot helped us to identify the stress overshoot as indicating yielding, whose characteristics obey some scaling laws. In step shear, contrary to the conventional perception that entangled polymers would undergo quiescent relaxation, the PTV observations reveal macroscopic motions after shear cessation [2]. The recoil-like macroscopic motions appears to reflect an elastic breakdown of the entanglement network due to sufficient build-up of retractive forces. LAOS experiments also demonstrate that entangled polymers cannot sustain a high magnitude of fast deformation without undergoing cohesive failure [3].


12:03PM J20.00005 Polymer Diffusion in Carbon Nanofiller / Polymer Nanocomposites. MINFANG MU, Department of Materials Science and Engineering, University of Pennsylvania, NIGEL CLARKE, Department of Chemistry, Durham University, RUSSSELL COMPOSTO, KAREN WINEY, Department of Materials Science and Engineering, University of Pennsylvania — Polymer tracer diffusion through carbon nanofiller / polymer nanocomposites is measured using elastic recoil detection methods. Tracer diffusion through a single wall carbon nanotube nanocomposite is strongly suppressed at low concentrations (≤ 0.4-0.8 vol%) and then increases at higher concentrations. In contrast, the typical Maxwell model predicts only a weak monotonic decrease. We propose a model for the carbon nanotube composite system wherein the SWCNTs function as cylindrical traps. Simulations of this model found that at low concentrations, the isolated traps retard polymer diffusion and at higher concentrations the percolated traps allow polymer diffusion to recover by providing continuous pathways. A comparison of our experimental and simulation results finds that (1) the strength of the trap increases with the molecular weight of the diffusing polymers and (2) the trap diameter increases with the molecular weight of the matrix polymer. Similarly, tracer diffusion through C60/polymer nanocomposites exhibits a significant decrease at low concentrations and then slowly increases at concentrations larger than 0.7 vol%.

12:15PM J20.00006 Tunable Wetting of Polymer Nanocomposite Films. MARLA MCCONNELL, SHU YANG, RUSSSELL COMPOSTO, University of Pennsylvania — Surfaces with controlled wettability are of growing technological importance. In this study, nanoparticles (NPs) with tunable spacing were assembled on poly(styrene-random-acrylic acid), S-r-AA, films to manipulate the composite films' wetting properties. Amine-modified silica NPs (15-200 nm) were covalently grafted to the AA moieties on the surface of the S-r-AA films, in which the S phase imparts mechanical stability and the AA domains swell, increasing the roughness and surface area. By controlling surface roughness and reaction time, NP coverage ranged from 1%-70%. These films displayed NP-coverage-dependent water contact angles between 60° and 120°. The enhanced hydrophobicity is attributed to capillary climbing of S-r-AA chains to cover the previously hydrophilic NP surface. Upon increasing NP diameter, the contact angle was found to increase at a fixed total coverage. This increase is attributed to the increase in effective surface area with increasing particle size. This system is utilized as a platform to create Janus particles with unique optical properties and templates for investigating molecular motors.
12:27PM J20.00007 Direct Measurement of Molecular Mobility in Actively Deformed PMMA Glasses

Hau-Nan Lee, Keewook Paeng, Stephen Swallen, Mark Ediger, Department of Chemistry, University of Wisconsin-Madison

To quantitatively understand the response of segmental motions to external stress, we performed optical measurements of dye reorientation in PMMA glasses during tensile creep deformation. Up to 1000-fold increases in mobility are observed during deformation, which supports the view that stress-induced mobility allows plastic flow in polymer glasses. Although the Eyring model describes this mobility enhancement well at low stress, it fails to capture the dramatic mobility enhancement after flow onset. In this regime, in addition to lowering the barriers for molecular motion, external stress apparently forces the shape of distribution of relaxation times to narrow significantly. The effect of stress on physical aging was also investigated. At low stress, physical aging and deformation-induced mobility act as two independent processes. However, after flow onset, the data are consistent with the view that aging has been erased by deformation.

12:39PM J20.00008 Probing Surface Glass Temperature of Polymer Films via Pentacene Growth Mode, Microstructure, and Thin-Film Transistor Performance

Choongik Kim, Antonio Facchetti, Tobin Marks, Northwestern University

Pentacene-based organic thin-film transistors (OTFTs) have been extensively studied in organic electronics. In this study, we report the fundamental importance of the polymeric gate dielectric glass transition temperature on pentacene film growth mode, and microstructure and corresponding OTFT performance. From the knowledge that nanoscopically-confined thin polymeric films exhibit glass-transition temperature deviations dictated from the corresponding bulk materials, we show here that pentacene films grown on polymeric gate dielectrics at temperatures well-below their bulk glass transition temperature ($T_g$) exhibit morphological/microstructural transitions and dramatic OTFT performance variations at a well-defined temperature [herein defined as the polymer surface glass transition temperature, or $T_g$($s$)] characteristic of the polymer structure and independent of the film thickness. Our results demonstrate that TFT measurements represent a new methodology to probe polymer surface viscoelastic properties.

12:51PM J20.00009 Responsive Polymer Surfaces: Crumpling, Folding, and Snapping Films

Douglas Holmes, Alfred Crosby

This work focuses on understanding deformation mechanisms and responsiveness associated with folding, crumpling, and snapping of thin polymer films attached to patterned and nonpatterned substrates. By studying folding and crumpling in confined regimes, we gain insight into material properties, while developing new strategies for adhesive, optical, and patterning applications. Using a novel processing technique, microarrays of freestanding polydimethylsiloxane plates are placed in equibiaxial compression and transition through crumpled morphologies that are difficult to attain through traditional patterning techniques. The microstructures also change their curvature through a snap-through instability via environmental stimuli. When triggered via osmotic pressure, the snap transition time scales as the square of the plate thickness and the inverse of the plate modulus. Recently, we have transferred this knowledge into the crumpling of ultrathin polymer films. We have fabricated sharply folded films directly on elastomeric and silicon substrates. The fold width scales directly with the film thickness and applied strain. We find that normally brittle, polystyrene films can accommodate excessive compressive strains without fracture by undergoing strain-localizing fold events.

1:03PM J20.00010 Structure and mobility of PEO/LiClO4 solid polymer electrolytes

Susan Fullerton, Janna Maranas, Penn State

Solid polymer electrolytes (SPEs) for use in rechargeable lithium-ion batteries offer many advantages over traditional liquid electrolytes, including mechanical flexibility and environmental friendliness. The practical limitation is that room temperature conductivity remains insufficient to power a portable device. While it is well-established that ion mobility is driven by polymer dynamics, high conductivity values have also been reported through fully crystalline SPEs. PEO-based SPEs have a rich phase behavior, and form several crystalline complexes depending on the lithium concentration, temperature, and recrystallization time. We investigate the structure, mobility, conductivity, and thermal properties of both semi-crystalline and amorphous PEO/LiClO4 SPEs. Structure is measured with small-angle neutron scattering, and PEO mobility with quasi-elastic neutron scattering. We observe a decoupling of ionic conductivity and PEO mobility in a semi-crystalline sample. We also determine that PEO atomic motion ahs undergone restricted rotation on a circle. The radius of the circle is consistent with a cylindrical, crystalline structure that persists to some extent in the amorphous phase. The results suggest that directed ion transport via ordered structures is perhaps equally important as polymer mobility for increasing conductivity, provided that the structures percolate over large spatial scales.

1:15PM J20.00011 Architectural effects in strongly hydrogen bonded thermoplastic elastomers

Kathleen Feldman, Craig Hawker, Edward Kramer, University of California, Santa Barbara

In this work we demonstrate the synthesis of random copolymers of n-butyl acrylate with a quadruple hydrogen bonding acrylate monomer based on 2-ureido-4-[1H]-pyrimidinone (UPy). Despite low $T_g$s and a lack of crystallinity, these materials show thermoplastic elastomer properties through the strong but thermoreversible UPy groups. Through the use of controlled radical polymerization and post-polymerization functionalization we are able to reach high UPy monomer content while maintaining low polydispersity and excellent control over the total molecular weight. It was found that the average distance between UPys along the chain was the major determiner of the overall properties including the plateau modulus, tensile modulus, and relaxation timescale. By using a difunctional initiator it is also possible to synthesize materials containing a homopolymer midblock and random copolymer end blocks, allowing us to address the question of how the MHB group distribution along the chain affects the bulk properties. In concentrating the UPy groups near the chain ends, the plateau modulus remained constant but the crossover frequency decreased. This knowledge was used to synthesize materials containing a homopolymer midblock and random copolymer end blocks, allowing us to address the question of how the MHB group distribution along the chain affects the bulk properties. In concentrating the UPy groups near the chain ends, the plateau modulus remained constant but the crossover frequency decreased. This knowledge was used to synthesize materials containing a homopolymer midblock and random copolymer end blocks, allowing us to address the question of how the MHB group distribution along the chain affects the bulk properties. In concentrating the UPy groups near the chain ends, the plateau modulus remained constant but the crossover frequency decreased, indicating that the effective lifetime of the hydrogen bonds within the supramolecular network increased, in keeping with prior theoretical predictions.
Measurements reveal a thermally activated increase in free carrier concentration for temperatures above 150 K, suggesting the presence of a defect level below the conduction band edge. In the present work, we used annealing to probe the influence of N interstitials on the electronic properties of GaAsN. In as-grown GaAsN films, temperature-dependent Hall fraction, presumably due to N diffusion to As vacancies. However, the influence of interstitial N on the electronic properties of GaAsN alloys remains unknown. In this contribution, we report newly performed first-principles calculations that clarify spin polarization and lattice relaxation of carrier concentrations with various charge states in a few group-III nitrides. Spin-polarized electronic configurations obtained in the present study are indicative of intrinsic ferromagnetism due to cation vacancies in nitride semiconductors.


1 Supported by NSF grant DMR-0802278

Effects of Si-N complexes on the electronic properties of GaAsN alloys

Influence of N Interstitials on the electronic properties of GaAsN Alloys

11:51 AM J21.00002 Interaction of hydrogen with defects in GaN

12:03 PM J21.00003 Intrinsic spin polarization of cation vacancies in group-III nitrides

12:27 PM J21.00005 N-H vibrational frequencies in GaAs:N:H

12:39 PM J21.00006 Effects of Si-N complexes on the electronic properties of GaAsN

1:15 PM J21.00007 Influence of N Interstitials on the electronic properties of GaAsN Alloys

We gratefully acknowledge the support of the National Science Foundation through a Focused Research Group (Grant No. DMR 0606406), monitored by Dr. LaVerne Hess.

We gratefully acknowledge the support of the National Science Foundation through a Focused Research Group (Grant No. DMR 0606406), monitored by Dr. LaVerne Hess.
1:03PM J21.00008 Quaternary Ga$_{1-x}$In$_x$P$_{1-y}$N$_y$ alloys described by clustering of In and N in GaP
Koushik Biswas, Alberto Franceschetti, Stephan Lany, National Renewable Energy Laboratory, Golden, CO — The interactions between the different atomic constituents in an alloy affect the microstructure, and ultimately, the electronic properties of the alloy. Specifically, in group III-V alloys the energy of formation of single defects and the binding energy of defect complexes play an important role in determining the microstructure. We present a model that starts from the dilute defect picture and extends to alloys of low to moderate concentrations. Using a valence-force-field (VFF) method we calculate the energy of formation of isolated N and In defects and that of small defect clusters formed by N and In in a GaP host. Considering a 1:2.12 N to In ratio that conserves lattice matching to GaP, we show that in a N concentration range up to ~15%, the formation energy of the random alloy can be described by the random probability to form such defect clusters. This approach allows the thermodynamic modeling of the microstructure of quaternary alloys, such as GaInNP, without intricate lattice-energy expansions and Monte-Carlo simulation techniques. In GaInNP, we find that short range ordering due to large atom to small atom preferential binding (i.e. In-N+GaP) strongly reduces the energy compared to the random distribution.

1:15PM J21.00009 Mechanism of Interaction between Hydrogen and the Two-dimensional Electron Gas in AlGaN/GaN High Electron Mobility Transistors
Jason Gu, Mahak Khandelwal, Jacob Melby, Carnegie Mellon University, Michael Steeves, University of Maine, Yuh-Renn Wu, Robert Lad, University of Maine, Robert F. Davis, Carnegie Mellon University — The large polarization difference between AlGaN and GaN causes a two-dimensional electron gas (2DEG) to form at the interface between the two semiconductors. Capacitance-voltage (CV) measurements revealed a charge density of 4.71x10$^{12}$ electrons/cm$^2$ in our 60 nm Al0.2Ga0.8N on 1.5 microns of GaN heterostructure. Exposure to hydrogen in the presence of a catalyst (Pt) resulted in a marked increase in the conductivity through the 2DEG. An interface state passivation mechanism is proposed as the most probable cause of this phenomenon. This mechanism was modeled using a self-consistent Schrödinger-Poisson solver, which showed that the passivation of interface states causes the shift of the Fermi level towards the conduction band, thereby increasing the carrier density of the 2DEG by 9%. In-situ CV measurements showed a 16% increase in the carrier density and a non-parallel shift in the CV curve when hydrogen was introduced, indicating a change in the number of available states. This supports interface state passivation as a cause of the increase in the conductivity through the 2DEG.

1:27PM J21.00010 Magnetodielectric coupling in Au/GaAs:Si Schottky barriers
S. Tongay, A.F. HEBARD, University of Florida, Y. HIKITA, H. HWANG, The University of Tokyo — A surprisingly large (>20%) negative magnetocapacitance in non-magnetic Au/GaAs:Si Schottky barriers is attributed to a magnetic field (H) induced increase in the binding energy of the shallow donor Si impurity atoms. Capacitance (C) dispersion is used to identify the impurity ionization and capture processes that give rise to an H-dependent density of ionized impurities N$_H$(H) in the depletion region. Internal photoemission experiments confirm that the large H-induced shifts in the built-in potential $V_{bi}$, inferred from Mott-Schottky (1/C$^2$ versus voltage) measurements, are not due to an H-dependent Schottky barrier height (SBH), thus requiring a modification of the abrupt junction approximation which identifies the dependence of $V_{bi}$ on N$_H$(H) rather than the SBH. The linearity of the Mott-Schottky plots is preserved, as experimentally observed. The underlying magnetodielectric coupling not only allows a new opportunity for the tuning of the dopant carrier density by an external means (magnetic field) but should be important for understanding the behavior of related interfacial structures incorporating dilute magnetic semiconductors and/or complex oxides.

1:39PM J21.00011 Point Defects and Dielectric Loss at MM Wavelengths in Wide-Gap Semiconductors
Jyotsna Dutta, Charles Jones, North Carolina Central University, V.V. Parshin, Applied Physics Institute, RAS, B. Garin, V.I. Polyakov, A. Rukovishnikov, Inst. of Radio Engineering and Electronics, RAS — Data are presented on wide-gap semiconductors of various grades for their dielectric loss values at millimeter wavelengths to explore their potential for various RF technology related applications. In order to identify the impurities or electrically active defects that give rise to the excess loss, temperature-dependent conductivity and DLTS measurements have been undertaken. Dielectric loss measurements over a wide range of temperatures are in progress to verify the results obtained from electrical methods and help to determine the primary loss mechanisms for these materials in the millimeter wave length range. Experimental results and their implications to loss properties will be discussed.

1:51PM J21.00012 Dual-Surfactant effect on enhancing different p-type doping in GaP
Junyi ZHU, Gerald Stringfellow, FENG LIU, University of Utah — We report first principles calculations demonstrating a dual-surfactant effect of Sb and H on enhancing Zn, Mg, Be and Cd in vapor phase epitaxially grown GaP thin films. The combined effects of Sb and H lower significantly the doping energy all the p-type dopants in GaP, while neither Sb nor H can work alone as effectively. The role of H is to satisfy the electron counting rule. The role of Sb is to serve as an electron reservoir to help electron redistribution. The enhancement is the lowest for Mg which is probably due to the lowest electronegativity of Mg among these four elements.

2:03PM J21.00013 InSb epilayers and quantum wells grown on Ge(001) substrates by MBE
Mukul Debnath, Tetsuya Mishima, Mike Santos, University of Oklahoma, Khalid Hossain, Wayne Holland, Amethyst Research Inc., University of Oklahoma Team, Amethyst Research Inc. Collaboration — For digital logic applications, transistors with both electron and hole channels are required. InSb:Ge heterostructures is an ideal material since the highest carrier mobilities for n and p-type quantum wells (QWs) are observed in InSb and Ge channels, respectively. We report on the MBE growth of InSb-based materials on Ge(001) substrates. A temperature variation two-step growth procedure (TSGP) is more effective than direct growth of InSb on Ge(001). In the TSGP, an initial 100-nm InSb layer was grown at a temperature of 340°C before increasing the substrate temperature to 420°C for the rest of the growth. The initial growth forms a wetting layer that minimizes defects at the InSb/Ge interface. The X-ray rocking curve width of a 5.0-µm-thick InSb epilayer is 173 arc sec. Electron mobilities of a 5.0-µm-thick InSb epilayer and an InSb/Al$_{0.2}$In$_{0.8}$/In$_x$P$_{1-x}$/GaAs QW at room temperature are 34,500 and 8,600 cm$^2$/V·s, respectively. These are the highest mobilities for an InSb epilayer and QW on Ge(001) substrates reported so far. This work was supported by NSF Grant DMR-0520550 and OCAST contract AR071-025.

Tuesday, March 17, 2009 11:15AM - 2:15PM — Session J22 GMAG DMP FLAP: Focus Session: Optical Control and Electron-nuclear Effects in Quantum Dots

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11:51AM J22.00002 Dynamical Nuclear Polarization via Triplet States in Self-Assembled Quantum Dot Molecules. S. C. BADESCU, D. KIM, A. S. BRACKER, D. GAMMON, T. L. REINECKE, Naval Research Laboratory, Washington DC — Recent experiments on self-assembled quantum dot molecules used molecular trion states to initialize and measure optically the electron spin in one of the dots [1]. The key to this experiment is the anticoating of two electron-triplet states in a magnetic field in Faraday configuration, which is due to spin-orbit coupling and electron-hole exchange. The experimental spin initialization and readout plots exhibit bifurcation and hysteresis features attributable to nuclear polarization. Here we present results for these effects from a model accounting for the feedback between the dynamical nuclear polarization and the electron spin states in the two dots, determined by the optical pumping and the asymmetric exchange. We explain the correlations between the nuclear polarizations in each of the dots and the asymmetry between the nuclear effects for the two measured electron states. [1] D. Kim et al, Phys. Rev. Lett. 101 (2008)

12:03PM J22.00003 Single frequency precession of inhomogeneous ensemble of electron spins. ALEX GREILICH, STEFAN SPATZEK, IRINA YUGOVA, ILJA AKIMOV, DMITRI YAKOVLEV, Experimental Physics 2, TU Dortmund University, Germany, ALEXANDER EFROS, Center for Computational Science, Naval Research Laboratory, Washington DC, USA, DIRK REUTER, ANDREAS WIECK, Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany, MANFRED BAYER, Experimental Physics 2, TU Dortmund University, Germany — We show that the spins of all electrons, each confined in a quantum dot of an (In,Ga)As/GaAs dot ensemble, can be driven into a single mode of precession about a magnetic field. This regime is achieved by allowing only a single mode within the electron spin precession spectrum of the ensemble to be synchronized with a train of periodic optical excitation pulses. Under this condition a nuclei induced frequency focusing leads to a shift of all spin precession frequencies into the synchronized mode. The macroscopic magnetic moment of the electron spins that is created in this regime precesses without dephasing. This ensemble can be used then as a macroscopic quantum bit.

12:15PM J22.00004 Control of the direction and rate of nuclear spin flips in InAs quantum dots using detuned optical pulse trains. SAM CARTER, SOPHIA ECONOMOU, Naval Research Laboratory, ANDREW SHABAEB, George Mason University, THOMAS KENNEDY, ALLAN BRACKER, THOMAS REINECKE, Naval Research Laboratory — Using two-color, time-resolved Faraday rotation and ellipticity measurements, we show that control of the direction and rate of nuclear spin flips in InAs quantum dots can be achieved through optical manipulation of the electron spin. A circularly polarized pump pulse train excites an ensemble of dots with varying electron spin precession frequencies and pump detunings. Resonant excitation has been described in Ref. [1], in which the electron spin polarization is greatly enhanced when the precession is synchronized to a multiple of the pulse repetition rate. Nuclear spin flips occur rapidly when the electron spin is not synchronized, with equal probability to flip up or down, leading to random walks that eventually lead the system to stable synchronized modes. In detuned dots, rotations of the spin away from the plane of precession lead to asymmetry in the nuclear spin flip rates, giving a clear pathway for nuclear reconfiguration. For dot energies below (above) the pump, the nuclear reconfiguration pushes electron spins towards (away from) synchronization. This effect is observed through a spectral shift in the Faraday rotation ellipticity amplitudes as a function of probe detuning. [1] A. Greilich, A. Shabaev et al., Science 317, 1896 (2007).

12:27PM J22.00005 Theory of the effect of detuned optical pulse trains on the electron-nuclear hyperfine interaction in quantum dots. SOPHIA ECONOMOU, SAM CARTER, Naval Research Lab, ANDREW SHABAEV, George Mason University, THOMAS KENNEDY, ALLAN BRACKER, TOM REINECKE, Naval Research Lab — A train of optical pulses detuned from resonance of the electron spin-trion transition in a quantum dot has the combined effect of generating and of rotating the spin polarization. The rotation is a direct consequence of the detuning and induces an electronic spin component parallel or antiparallel to the magnetic field, depending on the sign of the detuning. This electron spin component directs the nuclear spin to preferably flip in one direction. This pulse-assisted electron-nuclear flip-flop both affects the electron, because it changes the precession frequency and changes whether it is synchronized with the pulses, and it also opens up the opportunity for manipulating the nuclear polarization by using the detuning along with the pulse repetition rate as handles.

12:39PM J22.00006 Many-body theory of spin bath dynamics for qubit decoherence. REN-BAO LIU, WEN YANG, The Chinese University of Hong Kong — We have developed a cluster correlation expansion (CCE) theory for the many-body dynamics of a finite-size spin bath in a time scale relevant to decoherence of a center spin or a qubit embedded in the bath [1]. In terms of the linked cluster expansion, a cluster correlation term is the infinite summation of all the linked diagrams with all the spins in the cluster flip-flopped. The lowest order of the cluster correlation corresponds to the pair-correlation approximation developed previously [2]. In the thermodynamics limit, the CCE reduces to the standard cluster expansion. The CCE is especially useful for studying multi-spin interference in small spin systems such as NV centers in diamonds and molecular magnets, where the cluster expansion fails to converge to the exact solution.


This work was supported by Hong Kong RGC Project 401906.
12:51PM J22.00007 The Hyperfine-mediated and Nuclear-Dipolar-Induced Nuclear Spin. **EDDY YUSUF**, XUEDONG HU, Physics Department, University at Buffalo — We study nuclear spin diffusion in semiconductor quantum dots based on the density matrix approach. The nuclear spin interactions that we consider include both hyperfine-mediated and magnetic dipolar interactions. Furthermore, we take into account both the secular and the non-secular terms of the magnetic dipolar nuclear interactions. We discuss how the one- and two-electronic states in the quantum dots lead to quantitatively different nuclear spin polarization relaxation and nuclear spin diffusion time. We explore the behavior of the relaxation time and diffusion constant for various experimentally relevant parameters, and compare our results to the recently measured nuclear spin relaxation in GaAs double quantum dots [1].


1:03PM J22.00008 Theoretical study of the strain-induced nuclear spin depolarization in self-assembled quantum dots[1] . CHIA-WEI HUANG, XUEDONG HU, Department of Physics, University of Buffalo, SUNY Buffalo, NY 14260-1500 — We investigate how strain-induced quadrupole interaction is related to nuclear spin polarization in self-assembled quantum dots. Our calculation shows that the achievable nuclear spin polarization in In_{x}Ga_{1−x}As quantum dots is sensitively dependent on the strain distribution in the dots. There are two interesting regions of rapid changes in nuclear spin polarization when the Overhauser field is in the opposite direction to the external field. The first one occurs in the low field region (B < 1T) where nuclear spin polarization of individual nuclear species is suppressed due to a degeneracy between different nuclear spin states. The second one is a peak in nuclear spin polarization showing up in the intermediate field region. This peak corresponds to a local maximum of the Overhauser field, which happens when electronic Zeeman energy vanishes. Our results are in qualitatively agreement with the measured nuclear spin polarization in the experimental work of various groups.[2][3]

[1] We thank financial supports by NASA/LPS through ARO and NSF.

1:15PM J22.00009 Preparation of Nuclear Spin States in Double Quantum Dots[1]. JACOB J. KRICH, MICHAEL GULLANS, Harvard University, JACOB M. TAYLOR, MIT, MICHAEL STOPA, BERTRAND J. HALPERIN, MIKHAIL D. LUKIN, AMIR YACOBY, Harvard University — Recent experiments on double quantum dot systems with two electrons have shown rich dynamics associated with the hyperfine coupling to nuclear spins. We examine how the cycles used to produce dynamic nuclear polarization in such double quantum dots can lead to interesting non-equilibrium configurations of the nuclear spins. We develop a master equation for the nuclear spins, which we solve using time-dependent mean field theory. We find a rich set of phenomena in the system, including tendencies of the system to approach two very different configurations, one with equal effective magnetic fields produced by the nuclei in the two dots and the other with a large difference between the magnetic fields produced by the nuclei in the two dots, both of which are seen in experiments.

[1] This work has been supported in part by NSF grant DMR-0541988 and the Fannie and John Hertz Foundation.

1:27PM J22.00010 Zamboni force in pumping of angular momentum from electron to nuclear spins via the Overhauser effect. MICHAEL STOPA, AMIR YACOBY, JACOB KRICH, Harvard University — We identify a feedback mechanism between the electron states in a two-electron double quantum dot and the difference between the nuclear spin polarization in the two dots, which we term the “Zamboni force.” The Overhauser interaction is known to cause angular momentum transfer, spin flip-flops, between electrons and nuclei in GaAs-AlGaAs heterostructures. In double quantum dots, transport and pumping experiments have been performed to study the evolution of nuclear spin polarization in response to certain electronic transitions. We show that, in flipping from singlet (S) to triplet (T+), “flopping” of the nuclear spin can occur in the left dot, the right dot or in the barrier depending on the composition of the singlet state. Assuming a composite nuclear spin for each of the left dot, the right dot and the barrier, we numerically integrate the Schrödinger equation to study the gate voltage sweep through the S-T+ anti-crossing point. We show that the (nuclear) effective magnetic field gradient tends to produce spin flips in the dot with the weaker field and thereby constitutes a force toward nuclear spin equilibration.

1:39PM J22.00011 Spin Fluctuations in Magnetic Quantum Dots[1]. A.G. PETUKHOV, South Dakota School of Mines, R.M. ABOFATH, University of Texas, IGOR ZUTIC, SUNY Buffalo — We present a theoretical description of magnetism in quantum dots (QDs) doped with magnetic ions. It has been recognized that the mean-field theory (MFT) is inadequate for small magnetic systems, such as bound magnetic polarons (BMPs), at finite temperatures [1]. Magnetic QDs are in many respects similar to BMPs, however the latter are one-electron systems while the former may contain many electrons. Our approach requires the minimization of the generalized “free energy” functional [2] for QDs, which leads to a set of self-consistent Kohn-Sham-type equations that coincide with MFT-equations [3] in the thermodynamic limit. We reveal that the well-known spurious MFT second order phase transition in magnetization is completely removed by thermodynamic spin fluctuations.


3Supported by US ONR, NSF-ECCS.

1:51PM J22.00012 Carrier-mediated magnetism and bound magnetopolarons in quantum dots. RAFAL OSZWALDOWSKI, SUNY Buffalo and N. Copernicus University, Torun, Poland, ANDRE PETUKHOV, South Dakota School of Mines and Technology, Rapid City, IGOR ZUTIC, SUNY Buffalo — While Mn-doped quantum dots (QDs) offer versatile control of magnetic order [1], important challenges remain in understanding of these systems beyond the mean-field approximation. Furthermore, to describe the carrier-mediated magnetism in arrays of magnetic QDs and their non-equilibrium properties, it is important to consider the presence of both electrons and holes in these systems. We develop a formalism that accounts for both equilibrium and light-controlled magnetopolaron effects [2]. We study QDs of different sizes and find that their magnetic and photo-induced properties are extremely size-sensitive. We compare our theory with recent experiments on circularly-polarized photoluminescence in magnetic QDs [3] where both the magnetopolaron energies and power dependence of the circular polarization were measured. We thank I. R. Sellers for valuable discussions. Supported by ONR and NSF-ECCS CAREER. [1] L. Besombes et al., Phys. Rev. Lett. 93, 207403 (2004); R. M. Abolfath, A. G. Petukhov, and I. Zutic, Phys. Rev. Lett. 101, 207202 (2008); [2] T. Dietl and J. Spalek, Phys. Rev. Lett. 48, 355 (1982); [3] I. R. Sellers et al., unpublished.

2:03PM J22.00013 ABSTRACT WITHDRAWN —
11:15AM J23.00001 Coexistence of quantum phases in the quantum Hall regime of the 2$^{nd}$ Landau Level$^1$. TREVOR RHONE, JUN YAN, Columbia University, YANN GALLAIS, Université de Paris 7, ARON PINCZUK, Columbia University, LOREN PFEIFFER, KEN WEST, Alcatel-Lucent — We report the experimental study of spin excitation modes in the regime of quantum hall phases of the 2$^{nd}$ Landau Level. In the ferromagnetic state at $\nu=3$ the long wavelength spin wave mode is seen at the bare Zeeman energy. At low temperatures and at filling factors slightly lower ($\nu \sim 2.97$), the spin wave attenuates and a broad ‘overdamped’ continuum of low-lying excitations emerges. Under these conditions, sharp and broad modes coexist, suggesting the presence of mixed quantum phases. At slightly elevated temperatures the continuum disappears. Further away from filling factor three, near the odd-denominator state at $\nu \geq 8/3$, the continuum dominates at low temperature. However, the sharp spin wave is recovered at $T \geq 1K$. For even lower filling factors, such as $\nu \geq 5/2$, low temperature spectra display only the broad continuum of low-lying excitations. At high temperatures ($T \sim 2K$) a sharp spin wave is recovered while the broad continuum persists, indicating the emergence of phase coexistence. The interplay between sharp and ‘overdamped’ modes may manifest tendencies towards loss of full spin polarization in the $N=1$ Landau level and may indicate that spin degrees of freedom have significant impact on the physics of quantum Hall states with $3 \leq \nu \leq 2$.

$^1$Supported by NSF and DOE

11:27AM J23.00002 The Virtual Scanning Tunneling Microscope: Induced Tunneling in Bilayer Two-Dimensional Electron Systems. ADAM SCIAMBI, MATTHEW PELLICCIONE, DAVID GOLDBABER-GORDON, Stanford University, SETH BANK$^1$, ARTHUR GOSSARD, University of California, Santa Barbara, MICHAEL LILLY, JOHN RENO, Sandia National Laboratory — We propose a novel probe technique, the virtual scanning tunneling microscope (VSTM), which will spatially and spectroscopically map two-dimensional electron systems (2DESs) in semiconductor heterostructures. The probe overcomes the typical inaccessibility of a buried 2DES by having a second parallel “probe” 2DES grown nearby. A biased tip overhead can then induce local tunneling from the probe 2DES into the original by adjusting the interlayer potential barrier. Prior bilayer studies have shown that a tunneling signal is dominated by the overlap of the layers’ Fermi surfaces, hindering VSTM-induced tunneling and obscuring any spectroscopy. We show, however, in widely-space bilayers systems where interlayer inelastic scattering is more prominent that the previous energy-momentum constraints are relaxed. In GaAs/AlGaAs samples grown by different sources, we show we can increase interlayer tunneling by an order of magnitude with gating, setting the stage for spectroscopy.

$^1$Now with University of Texas at Austin.

11:39AM J23.00003 Tunneling spectroscopy of a 2D-2D tunnel junction: Towards a local spectroscopic probe of 2D electron systems. MATTHEW PELLICCIONE, ADAM SCIAMBI, DAVID GOLDBABER-GORDON, Stanford University, SETH BANK$^1$, ARTHUR GOSSARD, University of California, Santa Barbara, JOHN RENO, MICHAEL LILLY, Sandia National Laboratory — We present measurements on GaAs/AlGaAs bilayer two-dimensional electron systems (2DES) that exhibit inelastic tunneling between the 2D electron layers. Due to a relatively large interlayer separation, scattering allows for tunneling events between states of different energy and momentum, which are not observed in similar systems with a small interlayer separation. This behavior can be used to measure spectroscopic information about the 2DES that is obscured when tunneling events conserve energy and momentum exclusively. We study the bulk behavior of this system in the integer quantum Hall regime on samples from different sources, and provide a model to explain the observed tunneling dynamics. We also discuss the prospect of using this system as a virtual scanning tunneling microscope (VSTM), where a scanning probe is used to locally induce tunneling between the 2D electron layers.

$^1$Now with the University of Texas at Austin

11:51AM J23.00004 Unusual Cyclotron Resonance Line Broadening in Ultra-High Mobility Two-Dimensional Electron Gas System. LI-CHUN TUNG, NHMFL, CHANGLI YANG, Institute of Physics, Chinese Academy of Sciences, L.N. PFEIFFER, K.W. WEST, Bell Laboratories, Lucent Technologies, R.R. DU, Department of Physics and Astronomy, Rice University, YONG-JIE WANG, NHMFL — Microwave induced resistance oscillation in the ultra high mobility two-dimensional electron gas system has attracted an intense interest in recent years. Under the illumination of an intense microwave radiation in the millimeter regime, the system exhibits an unique resistance oscillation with a microwave-frequency-dependent period. We have carried out a FIR magneto-optical study up to 33T on a set of GaAs/AlAs ultra-high mobility heterostructure samples at 4K. At low magnetic field, ultra-sharp electron CR has been observed as expected. At high magnetic field, the halfwidth of CR grows rapidly with increasing magnetic field and this phenomenon is uniquely found in the 2DEG in the heterojunction. At the same time, there is no indication of a reduced mobility at high field in the transport measurement. The sudden broadening of the CR line shape cannot be simply interpreted by either the short- or long-range random potential. The halfwidth changes by at least an order, thus it can hardly be explained by either magnetophonon effect, inhomogeneity or magnetic oscillation.

12:03PM J23.00005 Evidence of Auger Satellite Lines in Landau-Level Photoluminescence Spectroscopy in a Two Dimensional Electron Gas$^1$. S.K. LYO, W. PAN, J.L. RENO, Sandia National Laboratories — Landau-level spectroscopy has provided a powerful tool for investigating the electronic structure and the scattering dynamics in a two-dimensional electron gas (2DEG) in the past. In this paper, we present theoretical and experimental evidence for Auger satellite lines in the magnetoluminescence of the Landau-level spectroscopy from a 2DEG under a perpendicular magnetic field $B$ at low temperatures. These new anomalous lines with a weak intensity appear below the energy gap in the form of radial “spokes” with negative slopes in the so-called fan (energy vs. $B$) diagram, in contrast to the well-known standard spokes of the fan diagrams of the spectral lines which appear above the band gap energy with positive slopes. [S. K. Lyo, E. D. Jones, and J. F. Klem, Phys. Rev. Lett. 61, 2265 (1988)]. Our theoretical predictions yield reasonable agreement with observed low-temperature data from GaAs quantum wells. The satellite lines can be used to determine the conduction (valence) band mass in n-doped (p-doped) systems.

$^1$Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. DOE under Contract No.DE-AC04-94AL85000.
of the conduction and valence band spin splittings. Since the electron g-factor value is known (1) in optical memories and computing, and in next generation of low-threshold optoelectronic devices.

1 We acknowledge the financial support of the Department of Energy, Office of Science, Basic Energy Sciences.

12:39PM J23.00008 Phase Separation of Bright and Dark Excitons in Coupled Quantum Wells

NICHOLAS SINCLAIR, ZOLTAN VOROS, JEFF WUENSCHELL, DAVID SNOKE, University of Pittsburgh, KENNETH WEST, LOREN PFIEFFER, Bell Labs — The diversity and complexity of solid-state environments suggests that Bose-Einstein Condensation (BEC) of excitations in a solid might manifest in a variety of interesting ways, in correspondence with the diversity of features around state of these systems. The pursuit of excitonic BEC is both enriched and obfuscated by this flexibility of condensate character. Previous research pursuing BEC of interwell excitons in GaAs coupled quantum wells (CQWs) has focused attention on observing unusual luminescence from ‘bright’, dipole-coupled (J=1) excitons to detect a BEC. However, theorists have recently predicted a ‘dark’ (J=2) ground state for interwell excitons in GaAs. Our recent work with interwell excitons confined in stress-induced, in-plane traps shows the critical onset of a dark spot in the exciton-recombination luminescence at trap center, suggestive of a dense population of dark excitons and a phase separation between the dark/bright species. The critical temperature vs. density in the low temperature regime matches well with ideal 2D harmonic trap BEC criteria, and preliminary theoretical work suggests that this degree of species separation cannot be explained by a model based on classical statistical level occupation using the bright/dark state energy separation.

12:51PM J23.00009 Ultrafast Relaxation Dynamics of a High Density Electron-Hole Plasma in High Magnetic Fields

JINHO LEE, DAVE H. REITZE, Physics Dept. University of Florida, JUNICHIRO KONO, Dept. of Electrical and Computer Engineering, Rice University, ALEXEY BELYANIN, Physics Dept., Texas A&M University, GLENN SOLOMON, NIST, STEVE MCGILL, NHMFL — We study the inter-Landau level relaxation dynamics of a dense electron-hole plasma in high magnetic fields (up to 31 T). Intense 150 fs pump pulses create carrier densities approaching 10^{13}/cm^2 in n_{GaAs}/GaAs multiple quantum wells. Relaxation dynamics are probed as a function of Landau level (LL) and magnetic field using time-resolved transient absorption (TRTA) and time-resolved photoluminescence (TRPL), which provide complementary information about the relaxation processes. Manifestly non-exponential decays of the TRTA signals are observed at high fields (above 15 T). TRPL emissions measured in the plane of the wells reveal the presence of multiple emission bursts from the LLs at high magnetic fields, suggesting a complicated relaxation process mediated by the field whereby carriers get trapped in a specific LL, emit PL through recombination, and then ‘reload’ as the carriers relax down to the previously occupied LLs.

1 Supported by the NSF through grant DMR-0325499 and by the NHMFL through an IHRP grant.

1:03PM J23.00010 Spin splitting of the valence band Landau levels in GaAs quantum wells

I. KHAN, T. ALI, M. YASAR, A. PETROU, SUNY at Buffalo, Buffalo NY, A. HANBICKI, G. KIOSEOGLOU, C. LI, B. JONKER, Naval Research Laboratory, Washington D.C. — We have studied as function of magnetic field the electroluminescence spectra from a n-i-p LED that incorporates three GaAs quantum wells in the intrinsic region. This device has excess n-type doping and as a result, the quantum wells are populated by a two-dimensional electron gas. The broad zero field emission band evolves into a series of discrete features in the presence of a magnetic field. These are identified as interband transitions between the f = 0, 1, and 2 Landau levels associated with the e_v and h_v subbands, with the selection rule \Delta f = 0. The EL spectra were analyzed in their \sigma+(LCP) and \sigma-(RCP) components. An energy splitting between the two polarized components is observed for each Landau level transition, which is equal to the sum of the conduction and valence band spin splittings. Since the electron g-factor value is known (g = -0.44) we were able to determine the valence band spin splittings. Our experimental values are compared to calculated values (1) and were found to be in reasonable agreement. Work at SUNY was supported by ONR and NSF 1. H.A. Nickel et al., Phys. Rev. B, 62, 2773, (2000)

1:15PM J23.00011 Bose Einstein Condensation in Trapped Polaritons Versus Lasing Effects

RYAN BALILI, BRYAN NELSEN, DAVID SNOKE, University of Pittsburgh, LOREN PFIEFFER, KENNETH WEST, Bell Labs, Lucent Technologies, UNIVERSITY OF PITTSBURGH TEAM, BELL LABS, LUCENT TECHNOLOGIES COLLABORATION — Evidence for Bose Einstein condensation (BEC) of exciton-polaritons have been presented recently by several groups in a variety semiconductor microcavity geometries (eg. [1]. Objections nevertheless remain as experimental evidence for polarization BEC bear striking similarity to observed behavior in a regular photon laser or micromaser in weak coupling regime. [2]. Latest results however show that a both BEC and lasing transitions can occur and are distinguishable in the stress trapped case [3].


1:27PM J23.00012 Optical Bistability in Coupled Microdisks

S.N. GHOSH, Y.K. VERMA, School of Natural Sciences, University of California, Merced, CA 95344, B.B. BUCKLEY, Department of Physics, University of California, Santa Barbara, California 93106, USA, X. LI, N. SAMARTH, Materials Research Institute, Penn State University, University Park, Pennsylvania 16802, USA, D.D. AWSCHALOM, Department of Physics, University of California, Santa Barbara, California 93106, USA, S. GHOSH, School of Natural Sciences, University of California, Merced, CA 95344, USA — Semiconductor microcavities offer unique means of controlling light-matter interactions in confined geometries, resulting in a wide range of applications in optical communications. We report bi-stable lasing in coupled GaAs microdisks with quantum wells and interface-fluctuation quantum dots in the active region. The inter-disk coupling results in mode-splitting, with the higher energy resonance persistently achieving higher mode Q (~ 4000). The bi-stability manifests in the form of hysteresis in the intensity of the coupled modes on non-uniform excitation and can be attributed to saturable absorption. This property in the lasing characteristics of coupled cavities gives us a control on the gain modulation and mode-switching and would be useful for applications in optical memories and computing, and in next generation of low-threshold optoelectronic devices.

1 This work was supported by NSF.
we study the polarization of the current as a function of the average spin orientation of iron atoms randomly dispersed over the nanotubes in a realistic setup. In particular, nanotube plus iron atom - has a magnetic moment of \(3\, \mu_B\) and recursive Green’s functions calculations we study the transport properties of disordered one-dimensional systems [1] composed of such units. In particular, nitrogen defects. We demonstrate that the Fe atoms bind to the four N defects in a configuration similar to a porphyrin molecule. Moreover, this system - CN sites of molecules, such as ammonia, and to be associated with the behavior of these sensors. In this work we study the adsorption of iron atoms onto these be used in a variety of nanoscopic electronic devices, and their functionality can be greatly enhanced by the introduction of defects. It has been shown that magnetic read-write heads. We report on the nano-electron beam assisted fabrication of atomically sharp iron-based tips and on the creation of a nano-soldering modify desired nanostructures for technological applications and to form molecular junctions and interconnections between carbon nanotubes. The development of the next generation of miniaturized electronic systems demands the integration of nanoelectronic components creating reliable mechanical and electrical contacts. At the same time, the development of scanning probe techniques and magnetic recording media require an ever decreasing tip size of ultrasharp magnetic read-write heads. We report on the nano-electron beam assisted fabrication of atomically sharp iron-based tips and on the creation of a nano-soldering iron for nano-interconnects using Fe-filled multiwalled carbon nanotubes (MWNTs). Our technique allows also carving a MWNT into a nanosoldering iron that was demonstrated capable of joining two separated halves of a tube. This approach could easily be extended to the interconnection of two largely dissimilar CNTs, between a CNT and a nanowire or between two nanowires.

11:51AM J24.00002 Carbon nanotube based sharp tips and soldering irons, ABHA MISRA, Graduate Aeronautical Laboratories (GALCIT), California Institute of Technology, Pasadena, CA, 91125, CHIARA DARAIO, Graduate Aeronautical Laboratories (GALCIT), and Applied Physics, California Institute of Technology, Pasadena, CA, 91125 — High energy electron beam machining has been proven a powerful tool to modify desired nanostructures for technological applications and to form molecular junctions and interconnections between carbon nanotubes. The development of the next generation of miniaturized electronic systems demands the integration of nanoelectronic components creating reliable mechanical and electrical contacts. At the same time, the development of scanning probe techniques and magnetic recording media require an ever decreasing tip size of ultrasharp magnetic read-write heads. We report on the nano-electron beam assisted fabrication of atomically sharp iron-based tips and on the creation of a nano-soldering iron for nano-interconnects using Fe-filled multiwalled carbon nanotubes (MWNTs). Our technique allows also carving a MWNT into a nanosoldering iron that was demonstrated capable of joining two separated halves of a tube. This approach could easily be extended to the interconnection of two largely dissimilar CNTs, between a CNT and a nanowire or between two nanowires.

12:03PM J24.00003 Broken chiral symmetry in nanotube sliding1, GIUSEPPE ERNESTO SANTORO, XIAOHUA ZHANG, International School for Advanced Studies (SISSA), UGO TARTAGLINO, Pirelli Tires, Milan, ERIO TOSATTI, International School for Advanced Studies (SISSA) — We discovered, in simulations of the frictional sliding of coaxial nanotubes, an unanticipated example of dynamical symmetry breaking – in fact a family of examples – taking place at the nanoscale. While both nanotubes are armchair, thus perfectly left-right symmetric and nonchiral, a nonzero angular momentum appears spontaneously at a series of critical sliding velocities, in correspondence with large peaks of the sliding friction. The angular momentum is not connected with real bodily rotations, but rather to breathing phonon pseudorotations. The nonlinear equations governing this phenomenon turn out to share common elements with another classical problem exhibiting a dynamical chirality breaking, that of forced oscillations of a string or a rope. Several new elements that are exquisitely “nano” appear in the nanotube case making it a richer, more elegant and intricate case, with a variety of different phenomena, and the crucial involvement of umklapp and of sliding nanofriction. 1This research was supported by Miur PRIN 2006022847 and by CNR/ESF/EUROCORES/FANAS/AFRI

12:15PM J24.00004 Porphyrin-like defects in CN\(_n\) nanotubes1, ANTONIO J.R. DA SILVA, Physics Institute - USP, JAMES ALMEIDA, A.R. ROCHA, Centro de Ciências Naturais e Humanas, UFABC, A. FAZZIO, Physics Institute - USP — Carbon nanotubes (CNT) can be used in a variety of nanoscopic electronic devices, and their functionality can be greatly enhanced by the introduction of defects. It has been shown that CNTs doped with nitrogen atoms can act as sensors. Pyridine–like defects, where four N atoms surround a divacancy, have been shown [1] to act as binding sites of molecules, such as ammonia, and to be associated with the behavior of these sensors. In this work we study the adsorption of iron atoms onto these nitrogen defects. We demonstrate that the Fe atoms bind to the four N defect in a configuration similar to a porphyrin molecule. Moreover, this system - CN\(_n\) nanotube plus iron atom - has a magnetic moment of \(3\, \mu_B\), which is almost entirely localized on the Fe atom. With a combination of density functional theory and recursive Green’s functions calculations we study the transport properties of disordered one-dimensional systems [1] composed of such units. In particular, we study the polarization of the current as a function of the average spin orientation of iron atoms randomly dispersed over the nanotubes in a realistic setup. 1A. R. Rocha, M. Rossi, A. Fazzio and A. J. R. da Silva, Phys. Rev. Lett. 100, 176803 (2008).

1We acknowledge support from FAPESP and CNPq.
12:27PM J24.00005 Dislocation Onset and Glide in Carbon Nanotubes under Torsion, TRAIAN DUMITRICEA, DONG-BO ZHANG, RICHARD JAMES, University of Minnesota — The torsional plastic response of carbon nanotubes is comprehensively described in the objective molecular dynamics framework [1-3]. It is shown that an (n,m) tube is prone to slip along a nearly-axial helical path, which introduces a distinct (+1,-1) change in the wrapping index. The low energy realization occurs without loss of mass, via nucleation of a 5-7-7-5 dislocation dipole, followed by a nearly-axial glide of the 5-7 dislocation. The onset of plasticity depends not only on chirality but also on handedness. For a given handedness of the applied twist, chiral tubes of opposed handedness are most susceptible to yield. A right-handed applied twist on an armchair (zig-zag) tube leads to a right- (left-) handed tube.


12:39PM J24.00006 Electrochemical Charging of Carbon Nanotubes for Tunable Field Emission Cathodes, ALEXANDER KUZNETSOV, NORMAN BARISCI, NanoTech Institute, University of Texas at Dallas, ANVAR ZAKHIDOV, ALEXANDER ZAKHIDOV, Cornell University, Ithaca, New York — Carbon nanotubes (CNTs) have very promising applications as electron field emitters. Work function of CNTs greatly affects the performance of such cold electron emitters. It is possible to change emission currents by several orders of magnitude by electrochemical charging. Electrochemical charging changes work function of CNTs by creating so called double layer. It was recently demonstrated that double layer structure remains for several hours after removing the CNTs from an electrolyte [1]. The extensive study of charging single wall carbon nanotube (SWNT) paper in different electrolytes has been performed at different charging potentials Vch. Field emission currents and threshold fields dependence on the charging potential and polarity is studied for various ions, with different valency and size: Na, Mg, Cs. Clear dependence of work function on Vch is demonstrated. AFM micro-imaging with a Kelvin probe allowed to study the micropatterns of work function modulation. Also dissipation of positive charge in air was investigated and its stability was significantly increased. 1. Suh Dong-Seok, Baughman Ray, Zakhidov Anvar, US Patent 20070170071 (2007)

12:51PM J24.00007 Interaction of water and methanol with graphene, C60 and (10,10) nanotube1, VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India, M. AMAR, Wright State Univ., J.F. MAGUIRE, Air Force Research Laboratory, Y. KAWAZOE, IMR, Tohoku Univ. Sendai, Japan — We study interaction of water and methanol molecules with graphene, C60 and (10,10) carbon nanotube using plane wave pseudopotential method and GGA. The interaction energies, ∆E, of H2O and CH3OH molecules on a (10,10) SWCNT, C60 and a graphene sheet are quite small (a few tens of meV) and are weakly dependent on the orientation of the molecules. The different electronic structures of graphene, nanotubes, and C60 lead to the differences. For (10,10) nanotube ∆E of water (39 meV) is favorable outside the nanotube and it increases for a water dimer. For methanol ∆E outside as well as inside the nanotube is nearly the same (40 meV). A competition between molecules-molecule and molecule-nanotube wall interaction could, however, lead to interesting molecular ordering behavior. ∆E of water on C60 is significantly smaller presumably due to its large HOMO-LUMO gap but for a graphene sheet the band gap vanishes and ∆E has an intermediate value between C60 and (10,10) nanotube. For methanol on graphene sheet ∆E increases to 60 meV due to more significant overlap of the molecular orbitals with those of the graphene sheet.

1Work supported by AOARD grant no. FA9550-05-P-0457.

1:03PM J24.00008 Hydrogen adsorption on metal coated Multiwalled Carbon nanotubes, XIANFENG ZHANG, DINESH RAWAT, TOYOHISA FURUHASHI, RAKESH SHAH, ALDO MIGONE, Department of Physics, Southern Illinois University at Carbondale, SAIKAT TALAPATRA — We present results of volumetric adsorption measurements of hydrogen, on Palladium-Gold (Pd-Au) coated multiwalled carbon nanotubes (MWNT). The nanotubes were prepared using air assisted chemical vapor deposition technique and were subsequently purified (acid treatment) before coating them with Pd-Au. Hydrogen adsorption measurements were performed at 77.3 K on as produced MWNTs as well as purified MWNT and compared with the adsorption isotherm obtained on Pd-Au coated MWNT samples under same experimental conditions. The effect of coating the MWNTs with Pd-Au on the adsorption behavior of hydrogen on these nanotubes will be discussed.

1:15PM J24.00009 Enhancement of In Vivo Anticancer Effect of Cisplatin by Incorporation Inside Carbon Nanohorns, MASAKO YUDASAKA, AIST, KUMIKO AJIMA, JST, TATSUYA MURAKAMI, YOSHIKAZU MIZOGUCHI, KUNIHIO TSUCHIDA, Fujita Health Univ., TOSHIHARI ICHIHASHI, NEC, SUMIO IIJIMA, JST, NEC, AIST, Meijo Univ. — We have been studying potential applications of single-wall carbon nanohorns (SWNHs) to drug delivery systems. SWNHs are multiply functionalized with proteins, magnetites, tumor targeting molecules, and others. Various drugs are easily incorporated, and the incorporated drugs are slowly released. Almost no acute toxicity of SWNHs was found through various animal tests. We show in this report that anticancer effect of cisplatin was enhanced by incorporation inside SWNHs (CDDP@SWNH) as evidenced by in vivo tests: CDDP@SWNH was locally injected to tumors subcutaneously transplanted on mice. CDDP@SWNH inhibited the tumor growth more effectively than CDDP. This anticancer enhancement was achieved by large CDDP-quantity incorporated inside SWNH, slow release of CDDP from SWNH, and a distinct (+1,-1) change in the wrapping index. The onset of plasticity depends not only on chirality but also on handedness. For a given handedness of the applied twist, chiral tubes of opposed handedness are most susceptible to yield. A right-handed applied twist on an armchair (zig-zag) tube leads to a right- (left-) handed tube.


1:27PM J24.00010 Fabrication of ZnPc/Protein Nanohorns for Double Photodynamic and Hyperthermic Cancer Phototherapy, MINFANG ZHANG, AIST, JST, TATSUYA MURAKAMI, Fujita Health Univ., KUMIKO AJIMA, JST, KUNIHIO TSUCHIDA, Fujita Health Univ., ATULA S. SANDANAYAKA, OSAMU ITO, Tohoku Univ., SUMIO IIJIMA, AIST, NEC, Meijo Univ., MASAKO YUDASAKA, AIST, JST, NEC — We developed double photodynamic and hyperthermic phototherapy systems [1] by loading zinc phthalocyanine (ZnPc) on single-wall carbon nanohorns (SWNHs). A protein of bovine serum albumin (BSA) was also attached to the surface of SWNHs. ZnPc performed photodynamic therapy (PDT) effect and SWNH had photothermogenic (PHT) effect. BSA endowed hydrophilic property to the system. Previous results in vitro showed that the efficiency of phototherapy using ZnPc-SWNH-BSA was higher than that of ZnPc or SWNHs. We show in this report that mouse tests also exhibited the similar tendency. ZnPc-SWNH-BSA was locally injected in tumors subcutaneously transplanted on mice. And the laser (670 nm) was irradiated for 15 minute everyday for 10 days. By this phototherapy, the tumors completely disappeared. The phototherapy using ZnPc or SWNHox-BSA exhibited weaker antitumor effects, and the tumors continued to grow. [1] Zhang et al. PNAS, 2008, 105, 14773.
1:39PM J24.00011 Terahertz Plasmon Oscillations at Room Temperature in Nanotube Transistors, DIEGO KIENLE, FRANÇOIS LÉONARD, Sandia National Laboratories, California — We present a theoretical study of the high-frequency properties of carbon nanotube transistors. We employ a new theory for AC quantum transport based on a self-consistent Non-Equilibrium Green Function formalism. The theory is applied to calculate the frequency dependent response of a semi-conducting \((17,0)\) nanotube FET device in the ballistic limit applying a time harmonic signal at the gate terminal. We show that in the ON-state the dynamical conductance exhibits divergent resonant peaks at discrete frequencies in the terahertz regime even at room temperature. These conductance peaks can be associated with the excitation of the charge eigenmodes (plasmons) of the quantum cavity formed by the nanotube channel and its surrounding gate, and shows up as pronounced spatial periodic large amplitudes in the AC charge and potential, respectively. The resonant features vanish when the device is operated in the OFF-state in which case the conductance displays smooth oscillations, a signature of single particle quantum interference. Our results indicate that low dimensional devices with nanometer channel length might show potential as novel detectors and emitters of THz radiation operating at room temperature.

1:51PM J24.00012 Effects of substrate relaxation on adsorption in pores, SILVINA GÁTICA, Howard University, HYE-YOUNG KIM, Southeastern Louisiana University, GEORGE STAN, University of Cincinnati, MILTON COLE, Pennsylvania State University — Fluids in porous media are commonly studied with analytical or simulation methods, usually assuming that the host medium is rigid. Large qualitative effects are found for several systems, for which substrate relaxation may not be neglected. One application is a determination of the ground state of 3He in slit and cylindrical pores, where the relaxation effects vanish when the device is operated in the OFF-state in which case the conductance displays smooth oscillations, a signature of single particle quantum interference. Our results indicate that low dimensional devices with nanometer channel length might show potential as novel detectors and emitters of THz radiation operating at room temperature.


11:15AM J25.00001 Quantum and transport scattering times in graphene, X. HONG, K. ZOU, J. ZHU, Department of Physics, Penn State University, A. POSADAS, J. HOFFMAN, C. H. AHN, Department of Applied Physics, Yale University — We study the quantum\((\tau_q)\) and transport\((\tau_t)\) scattering times of single layer graphene mechanically exfoliated on SiO\(_2\) and polycrystalline Pb(Zr,Ti)O\(_3\) (PZT) substrates. The PZT substrate exhibits a gating efficiency of \(2 \times 10^{11}\,\text{cm}^2/\text{V} \times \text{s}\), corresponding to a dielectric constant of \(\sim 12\). We extract \(\tau_q\) from the magnetic field dependence of Shubnikov de Haas oscillations and \(\tau_t\) from the zero gate mobility, respectively. For the PZT-gated graphene, in the density range of \(2 \times 10^{12}/\text{cm}^2 < n < 6 \times 10^{12}/\text{cm}^2\), the transport scattering time \(\tau_t\) exhibits a clear crossover from a \(n^{1/2}\) dependence to a very weak density dependence at \(n \approx 4 \times 10^{12}/\text{cm}^2\). This observation is consistent with the theoretical prediction of a transition from long to short-ranged impurity scattering in graphene. On the other hand, the quantum relaxation time \(\tau_q\) shows a \(n^{1/2}\) dependence for the whole carrier density range. The ratio \(\tau_q/\tau_t\) changes from 2.5 to 1.8. Similar measurements are carried out on SiO\(_2\)-gated graphene. We compare data obtained from both substrates.

11:27AM J25.00002 Electrical and structural properties of chemically modified graphene sheets, ANDREA C. FERRARI, University of Cambridge, Engineering Department, Cambridge, CB3 OFA, UK — The chemical exfoliation of graphite through oxidation and then dispersion in a solvent is one of the methods of achieving scalable production of single graphene sheets. We use this method for making chemically modified graphene (CMG) sheets with tunable electronic properties, which can be placed flat on any surface or dispersed in various matrices. CMG sheets share some similarities with pristine graphene and with carbon nanotubes, e.g. tunable electron- and hole-type conductivity is observed in single CMG sheets just above the percolation threshold. CMGs may also be considered as a template for a bottom up development of a new class of materials. We have performed electrical measurements of individual CMG sheets and will discuss their electronic properties and the possible mechanisms of the charge transport in relation to their atomic structure and chemical composition.

11:39AM J25.00003 Doping, Strain, Orientation and Disorder of Graphene by Raman Spectroscopy, ANDREA C. FERRARI, University of Cambridge, Engineering Department, Cambridge, CB3 OFA, UK — Raman spectroscopy is a fast and non-destructive method for the characterization of carbons [1]. These show two features: the G and D peaks, around 1580 and 1350 cm\(^{-1}\), respectively. The G peak corresponds to the doubly degenerate \(E_2g\) phonon at the Brillouin zone centre. The D peak is due to the breathing modes of sp\(^2\) atoms and requires a defect for its activation [1-5]. It is common for as-prepared graphene not to have enough structural defects for the D peak to be seen [4,6], so that it can only be detected at the edges [6]. The most prominent feature in graphene is the second order 2D peak [6]. This is always seen, since no defects are required for its activation. Its shape changes single and multi-layers [6]. Raman spectroscopy also monitors doping [7-9]. We report the evolution of the Raman spectra of single [7,9] and bi-layer [9] graphene as a function of doping. A Fermi level shift is induced either by applying a bottom gate [7], or by a polymeric top gate [8,9], or naturally happens as a result of charged impurities [7]. This induces a stiffening of the Raman G peak for both hole and electron doping [7]. This is explained, including dynamic corrections to the adiabatic Born-Oppenheimer approximation [7]. The phonon renormalization of bilayer graphene has characteristic features compared to single layer. This allows a direct estimation of the interlayer coupling [7-9]. We then consider the effects strain. Uniaxial strain lifts the \(E_2g\) degeneracy and splits the G peak in two: \(G^+\) and \(G^-\). The peaks downshift as a function of strain allows a direct measurement of the Gruneisen parameter [10]. The polarization dependence of the \(G^+/G^-\) mode is a probe of the crystallographic orientation of the sample [10]. Finally, we consider the effect of disorder [3,4,11] and show how to discriminate between disorder, strain and doping [11]. We will also discuss how the D peak is a signature of \(\pi\) electron localisation, and thus, of gap opening in chemically modified graphene [12].
transport properties of epitaxial graphene on Si-face SiC and 3-inch SiC wafers, an agenda that we are now pursuing.

12:27PM J25.00005 Frictional Characteristics of graphene, CHANGGU LEE, Columbia University, ROBERT CARPICK, University of Pennsylvania, JAMES HONE, Columbia University — The frictional characteristics of graphene were characterized using friction force microscopy (FFM). The frictional force for monolayer graphene is more than twice that of bulk graphite, with 2,3, and 4 layer samples showing a monotonic decrease in friction with increasing sample thickness. Measurements on suspended graphene membranes show identical results, ruling out substrate effects as the cause of the observed variation. Likewise, the adhesion force is identical for all samples. The frictional force is independent of load within experimental uncertainty, consistent with previous measurements on graphite. We consider several possible explanations for the origin of the observed thickness dependence.

12:39PM J25.00006 Using Defects as Local Electronic Probes of Epitaxial Graphene on SiC, GREGORY M. RUTTER, KEVIN D. KUBISTÅ, DAVID L. MILLER, MING RUAN, WALTER A. DE HEER, PHILLIP N. FIRST, School of Physics, Georgia Institute of Technology, Atlanta, GA, JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD — Defects play an important role in the transport properties of epitaxial graphene, and understanding this role is essential for realizing potential nanoelectronics based on graphene. In this study, scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) performed at 4.2 K are used to measure the local electronic behavior of defects in epitaxial graphene grown on both SiC(0001) and SiC(000-1). Energy-resolved maps of the differential conductance reveal defect-induced standing-wave modulations related to the unique nature of the graphene band structure. In this talk, I will discuss how these defects can be used as a local probe of the graphene electronic properties with the inclusion of an applied magnetic field and the resulting Landau quantization. Supported in part by NSF, NRI-INDEX, and the W. M. Keck Foundation.

12:51PM J25.00007 ABSTRACT WITHDRAWN —

1:03PM J25.00008 Crystallographic Cuts in Single Layer Graphene, LEONARDO CAMPOS, VITOR MANFRINATO, JAVIER SANCHEZ, JING KONG, PABLO JARILLO-HERRERO, MIT — Graphene consists of a single monolayer of carbon atoms in a honeycomb 2D crystal. It is unique because the electrons are described by the Dirac equation, like relativistic particles with zero rest mass. According to theoretical predictions, it is possible to create field effect transistors just using narrow (d<10nm) nanoribbons. With zigzag edges, graphene nanoribbons can have a large magneto-resistance or could be used to produce a spin valve. With armchair edges it is possible to have an energy gap controllable by electric field. In this work we will show how to use Ni nanoparticles to create crystallographic oriented cuts in exfoliated graphene. Using Raman spectroscopy and electronic measurements of Dirac peaks, we have verified that the graphene, after the high temperature nanocut etching process, are still high quality 2D crystals, indicating that this process can be used to produce graphene nanodevices. Using this method we fabricate oriented nanoribbons and equilateral triangles with varying size. We also present a detailed analysis of the fabrication conditions for controlling the etching characteristics. Last, we present our analysis of the chirality of our nanocuts.

1:15PM J25.00009 Chiral tunneling of Dirac electrons in strained graphene, A. GARCIA-SARAVIA, G. CORDOURIER-MARURI, M.E. CIFUENTES-QUINTAL, E. MARTINEZ-GUERRA, R. DE COSS, Departamento de Fisica Aplicada, CINVESTAV-Mérida, A. P. 73 Cordemex, Mérida, Yucatan, Mexico — The behavior of the electrons in graphene is like massless Dirac fermions, which is a consequence of the characteristic energy spectrum of this material (E= k). Perfect chiral tunneling is expected when Dirac electrons pass through a step barrier (Klein paradox). However, in a two-dimensional system like graphene, the perfect tunneling is obtained only in a small range of incident angles. In the present work, we have studied the uniaxial deformation as a method of tuning the electronic transmittance in graphene. The effect of the armchair and zigzag strain on graphene was studied by means of first principles calculations, using the Density Functional Theory. For the calculations we used the pseudopotential-LCAO method. We found that the uniaxial deformations, induce an ellipsoidal distortion of the Dirac cones and isotropy breaking of the Fermi velocity. Finally, we used the Dirac–like equation to model the electronic transmittance as a function of the incident angle. We obtain that the strain induces a strong changes in the transmittance when the deformation is perpendicular to the incident axis.

1:27PM J25.00010 Strain and adhesion of graphene sheets in shallow trenches, CONSTANTZ METZGER, SEBASTIAN REMI, SILVIA KIJSMINSKY, ANTONIO CASTRO NETO, ANNA SWAN, BENNETT GOLDBERG, Boston University — Detailed high resolution micro Raman mapping of graphene exfoliated over shallow trenches demonstrates that single layer graphene adheres to the bottom of shallow trenches instead of remaining freely suspended. The analysis shows that the strain is surprisingly uniform. The high resolution Raman mapping of G and 2D Raman modes are consistent with uniaxial strain measurements, and the strain map concurs with our theoretical calculations that predict that a graphene sheet reaches minimal free energy sticking to the trench bottom even if that leads to moderate strain of about 0.6% in the sheet.

1:39PM J25.00011 ABSTRACT WITHDRAWN —

1:51PM J25.00012 Correlation of optical and topographical measurements with electronic transport properties of epitaxial graphene on Si-face SiC, PAUL M. CAMPBELL, Naval Research Laboratory, Washington DC, JOSHUA ROBINSON, Pennsylvania State University, University Park PA, JAMES C. CULBERTSON, JOSEPH L. TEDESCO, ROY A. MABOUDIAN, CARLO CARRARO, University of California at Berkeley, JASON KAWASAKI, Princeton University, ROYA MABOUDIAN, CARLO CARRARO, University of California at Berkeley — The early stages of epitaxial graphene layer growth on the Si-terminated 6H-SiC(0001) are investigated by depolarized Raman spectroscopy and electron channeling contrast imaging. The selection of the depolarized component of the scattered light results in a significant increase in the C=C bond signal over the second order SiC Raman signal, which allows us to resolve submonolayer growth, the formation of the buffer layer and a strained graphene layer. The linear strain, measured at room temperature (RT), is found to be compressive, which can be attributed to the large difference between the coefficients of thermal expansion of graphene and SiC. Whereas film thickness is determined by growth temperature, both the magnitude of the compressive strain and film morphology can be varied by adjusting the growth time at fixed annealing temperature. Annealing times in excess of 8-10 minutes lead to an increase in the mean square roughness of SiC step edges to which graphene films are pinned, resulting in compressively stressed films at RT. Shorter annealing times produce minimal changes in the morphology of the terrace edges and result in nearly stress-free films under cooling to RT.

1:51PM J25.00014 Controlled Structural Strain in Epitaxial Graphene Layers on 6H-SiC and Effects on Surface Morphology, NICOLA FERRALIS, University of California at Berkeley, JASON KAWASAKI, Princeton University, ROYA MABOUDIAN, CARLO CARRARO, University of California at Berkeley — The early stages of epitaxial graphene layer growth on the Si-terminated 6H-SiC(0001) are investigated by depolarized Raman spectroscopy and electron channeling contrast imaging. The selection of the depolarized component of the scattered light results in a significant increase in the C=C bond signal over the second order SiC Raman signal, which allows us to resolve submonolayer growth, the formation of the buffer layer and a strained graphene layer. The linear strain, measured at room temperature (RT), is found to be compressive, which can be attributed to the large difference between the coefficients of thermal expansion of graphene and SiC. Whereas film thickness is determined by growth temperature, both the magnitude of the compressive strain and film morphology can be varied by adjusting the growth time at fixed annealing temperature. Annealing times in excess of 8-10 minutes lead to an increase in the mean square roughness of SiC step edges to which graphene films are pinned, resulting in compressively stressed films at RT. Shorter annealing times produce minimal changes in the morphology of the terrace edges and result in nearly stress-free films upon cooling to RT.
2:03PM J25.00013 Reconstruction of Vacancy Defects in Graphene and Carbon Nanotube
GUN-DO LEE, EUJOOON YOON, NONG-MOON HWANG, Seoul National University, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University — Recently, various structures of vacancy defects in graphene layers and carbon nanotubes have been reported by high resolution transmission electron microscope (HR-TEM) and those arouse an interest of reconstruction processes of vacancy defects. In this talk, we present reconstruction processes of vacancy defects in a graphene and a carbon nanotube by tight-binding molecular dynamics (TBMD) simulations and by first principles total energy calculations. We found that a structure of a dislocation defect with two pentagon-heptagon (5-7) pairs in graphene becomes more stable than other structures when the number of vacancy units is 10 and over. The simulation study of scanning tunneling microscopy reveals that the pentagon-heptagon pair defects perturb the wavefunction of electrons near Fermi level to produce the \( \sqrt{3} \times \sqrt{3} \) superlattice pattern, which is good agreement with experiment. It is also observed in our tight-binding molecular dynamics simulation that 5-7 pair defects play a very important role in vacancy reconstruction in a graphene layer and carbon nanotubes.

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J26 DMP DCOMP: Focus Session: Computational Nanoscience IV: Carbon- and Silicon-based Nanostructures 328

FENG LIU, University of Utah — The nanotechnology of the future demands controlled and consistent fabrication of different classes of nanostructures. Computational nanoscience can play an important role in the development of novel nanofabrication techniques. By revealing the fundamental differences in the mechanical bending behavior of nanofilms from that of micro- and macro-films, we have carried out atomistic simulations making significant contributions to advance a novel nanofabrication approach, the so-called “nanomechanical architecture” of thin films. This approach allows fabrication of different types of nanostructures, with a high level of control over their size and shape based on a priori theoretical/computational designs. The simulations have revealed a self-bending mechanism of Si (Ge) nanofilms leading to formation of pure Si (Ge) nanotubes, which greatly broadens the repertoire of nanotubes that can be made from multilayer films. Furthermore, applying the principle of nanomechanical architecture to the extreme case of the thinnest film possible, a single atomic layer of patterned graphene sheet, a new method for synthesizing carbon nanotubes with an unprecedented control over their size and chirality was proposed.

12:03PM J26.00007 Thermal activation of interlayer bonding and its effect on properties of multiwalled carbon nanotubes
CHUN TANG, Department of Physics & High Pressure Center, University of Nevada, Las Vegas, WANLIN GUO, Institute of Nano Science, Nanjing University of Aeronautics & Astronautics, CHANGFENG CHEN, Department of Physics & High Pressure Science and Engineering, University of Nevada Las Vegas — We report molecular dynamics simulations of multiwalled carbon nanotubes (MWCNTs) at high temperatures. Our results show that thermally activated interlayer bonding have significant influence on structural, mechanical and electronic properties of MWCNTs and lead to new behaviors with implications for their applications. We examine the effect of strain and temperature conditions on the formation of interlayer bonding in MWCNTs and unveil the underlying atomistic mechanisms.

12:15PM J26.00004 Effective Hamiltonian approach to bright and dark excitons in single-walled carbon nanotubes
SANGKOOK CHOI, JACK DESLIPPE, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Recently, excitons in single-walled carbon nanotubes (SWCNTs) have generated great research interest due to the large binding energies and unique screening properties associated with one-dimensional (1D) materials. Considerable progress in their theoretical understanding has been achieved by studies employing the ab initio GW-Bethe-Salpeter equation methodology. For example, the presence of bright and dark excitons with binding energies of a large fraction of an eV has been predicted and subsequently verified by experiment. Some of these results have also been quantitatively reproduced by recent model calculations using a spatially dependent screened Coulomb interaction between the excited electron and hole, an approach that would be useful for studying large diameter and chiral nanotubes with many atoms per unit cell. However, this previous model neglects the degeneracy of the band states and hence the dark excitons. We present an extension of this exciton model for the SWCNT, incorporating the screened Coulomb interaction as well as state degeneracy, to understand and compute the characteristics of the bright and dark excitons, such as the bright and dark level splittings. Supported by NSF #DMR07-05941, DOE #DE-AC02-06NA26274 and computational resources from Teragrid and NERSC.

12:27PM J26.00005 First-principles studies of the optical properties of carbon nanohoops
JOYDEEP BHATTACHARJEE, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory — First proposed 70 years ago, cycloparaphenylenes — cyclic aromatic molecules that are the shortest possible segment of an armchair nanotube — have been only recently synthesized [1]. Using first-principles density functional theory and a Bethe-Salpter equation approach, we study structural, electronic, and optical properties of this novel class of materials, coined "carbon nanohoops." Remarkably, we find, in agreement with experiments, that smaller hoops have smaller optical absorption gaps. This counterintuitive trend, opposite to that expected from ordinary quantum confinement, reflects a large increase in electron-hole interaction strength with decreasing hoop diameter. The diameter dependence of this interaction is thoroughly explored for several nanohoops, compared with an acyclic series, and discussed in the context of possible applications. [1] R. Jasti, J. Bhattacharjee, J. B. Neaton, and C. R.Bertozzi, submitted (2008).

1This work was supported in part by the NCN through the NSF and U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
12:39PM J26.00006 First-principles study of methane adsorption on defective graphitic nanomaterials. BRANDON WOOD, Theoretical Sciences Unit, JNCASR, Bangalore, India, DEBOSRUTI DUTTA, MANAPATHY AYAPPA, Department of Chemical Engineering, Indian Institute of Science, Bangalore, India, SHOBHANA NARASIMHAN, Theoretical Sciences Unit, JNCASR, Bangalore, India — Efficient storage of methane represents a significant challenge to large-scale implementation of natural gas-based consumer transportation. Activated carbons and related carbon-based nanoporous structures have garnered tremendous interest as storage media due to their unusually high absorptive capacities. However, systematic improvement of these materials relies on a fundamental understanding of the physical and chemical processes involved. We present here extensive energetic calculations of methane adsorption in model carbonaceous systems using density-functional techniques. As exact nanostructures of activated carbons are difficult to obtain, we have attempted to isolate likely model nanostructures and defects, including surfaces, edges, point defects, and chemical functionalization. For each of these cases, we analyze changes in the structural, magnetic, and electronic properties upon adsorption. The defect structures exhibiting strongest methane adsorption are isolated, and the relevant mechanisms dominant in binding are identified. The impact of our results in terms of increasing methane absorptive capacity in activated carbons is discussed.

12:51PM J26.00007 Effects of hydrogen chemisorption on the structure of carbon nanotubes. ANDRE MUNIZ, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts at Amherst — We report results of a computational atomic-scale analysis of the effects of atomic hydrogen chemisorption on the structure of single-walled and multi-walled carbon nanotubes (SWCNTs and MWCNTs). The analysis combines classical molecular-dynamics simulations with first-principles density functional theory calculations. We find that H chemisorption induces structural changes in SWCNTs associated with sp²-to-sp³ bonding transitions; increasing the H coverage beyond a critical level leads to axial and radial expansion of the SWCNTs that increases monotonically with H coverage. We also investigated the possibility of H-induced inter-shell sp³ C-C bond formation in MWCNTs. We find several pathways that lead to stable inter-shell bonded structures, which can act as seeds for nucleation of various crystalline carbon phases embedded into the MWCNTs. Finally, we show how the chiralities and relative alignments of adjacent graphene walls in MWCNTs determine the resulting crystalline structures.

1:03PM J26.00008 First principles study of NH₃ adsorption on carbon nanowires. JORGE-ALEJANDRO TAPIA, ALVARO-DANIEL SANCHEZ, CESAR ACOSTA, Facultad de Ingeniería (UADY), GABRIEL CANTO, Centro de Investigaciones en Corrosion (UACAM) — Recently has been reported a new type of one-dimensional carbon structures. Carbon nanowires formed by a linear carbon-atom chain inside an armchair (5,5) carbon nanotube has been observed using high-resolution transmission electron microscopy. Theoretical and experimental studies of the NH₃ adsorption in the carbon nanotubes report changes in the electronic properties of the carbon nanotubes. In the present work we have studied the electronic and structure properties of carbon nanowires (chain@SWCNT) when NH₃ atoms are adsorbed. We used the Density Functional Theory and the calculations where performed by the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We have analyzed the changes in the atomic structure and density of states (DOS). We found that the electronic character of the carbon chain of the chain@SWCNT system can be modulated by NH₃ adsorption. This research was supported by SEP under Grant No. PROMEP/103.5/07/2595 and the Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grants No. 82497 and 60534.

1:15PM J26.00009 First-Principles Studies of Octacyclopropylcubane: A Novel High-Energy Density Material. STEVEN L. RICHARDSON, Howard University, REESHEMAH N. ALLEN, DANIEL FINKENSTADT, Naval Research Laboratory, MICHAEL J. MEHL, MARK R. PEDERSON, Naval Research Laboratory — The ongoing quest for synthesizing novel high-energy density materials (HEDMs) is clearly motivated by a search for new propellants and explosives. Recently de Meijere et al. have synthesized a new HEDM, octacyclopropylcubane (C₃₂H₄₀), in which the eight hydrogen atoms of cubane were replaced by cyclopropyl groups. In this work we report the results of a first-principles density-functional theory (DFT) calculation using the suite of codes known as NRLMOL (Naval Research Laboratory Molecular Orbital Library) to compute the structural, electronic, and vibrational properties of octacyclopropylcubane. We have calculated the vibrational properties of C₃₂H₄₀ and compare our results with experiment. We have also employed a DFT-based tight-binding scheme to compute the vibrational density of states for octacyclopropylcubane and compare our results with our full DFT-based results. Interesting enough, the geometry of the cyclopropyl groups in C₃₂H₄₀ does not allow for the quartic- concerted torsional mode (QCTM) that we and other workers have previously studied in octanitrocubane.

1:27PM J26.00010 Efficient first-principles simulation of non-contact atomic force microscopy for structural analysis. JAMES CHELIKOWSKY, TZU-LIANG CHAN, University of Texas at Austin, CAIL-ZHUANG WANG, Ames Laboratory-U.S. DOE, KAI-MING HO, Iowa State University — Non-contact atomic force microscopy (nc-AFM) has made significant advances that have allowed one to image a surface at atomic resolution. However, first-principles simulations of nc-AFM images remain a challenge because they involve calculations of the sample together with an atomic model of the AFM tip. We propose an efficient scheme to simulate nc-AFM images by using a first-principles self-consistent potential from the sample as input and without explicit modeling of the AFM tip. Our method is applied to various types of semiconductor surfaces including Si(111) (7 x 7), TiO₂(110) (1 x 1), Ag/Si(111)-(√3 x √3)/R30°, and Ge/Si(105) (1 x 2) surfaces. Our method takes into account electronic effects of the tip-sample interaction, which are important for predicting the bright spot positions and the contrast change with AFM tip height. In addition, we obtain good agreement with experimental results and previous theoretical studies.

This work was supported by the National Science Foundation under DMR-0551195 and the U.S. DOE under DE-FG02-06ER46286 and DE-FG02-06ER15760.

1:39PM J26.00011 Ab initio calculation of Stokes shifts of hydrogenated silicon clusters. MARIE LOPEZ DEL PUERTO, University of St. Thomas, St. Paul, MN, MANISH JAIN, University of California, Berkeley, CA, JAMES R. CHELIKOWSKY, University of Texas, Austin, TX — There is experimental evidence that hydrogenated silicon clusters may have large Stokes shifts. The absorption and emission processes in these clusters are not symmetric because the clusters may undergo structural changes while in an excited state. Several theoretical methods have been used to study this problem, resulting in an array of predicted Stokes shifts that differ in energy by several eVs, and different predicted minimum-energy structures with either relaxed cores or relaxed outer shells. We calculate Stokes shifts using three different methods: density functional theory within the local density approximation (LDA), density functional theory within the generalized gradient approximation (GGA), and time-dependent density functional theory within the local density approximation (TDLDA). We find that these three different methods give similar results both for magnitude of Stokes shift and excited-state structures. The Stokes shift of hydrogenated silicon clusters of 5 to 35 silicon atoms range from 5.5eV to 0.8eV, decreasing with increasing cluster size.

This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.
1:51PM J26.00012 Calculated Polarizabilities of Diamond and Silicon Nanoclusters¹. SUDHA SRINIVAS, Physics Department, Northeastern Illinois University, Chicago, IL 60625, KOBLAR JACKSON, Physics Department, Central Michigan University, Mt. Pleasant, MI 48859, MINGLI YANG, Institute for Nanobiomedical Technology and Membrane Biology, Sichuan University, Chengdu 610041, China, JULIUS JELLINEK, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 — A scheme for decomposing the electric polarizability of a system into site-specific contributions is applied to hydrogenated nanoclusters of carbon and silicon. Site-specific dipole moments and polarizabilities are obtained from the response of charge densities to external electric fields, and decomposed into local and charge transfer components. We study changes in the polarizabilities of the C and Si atoms as the clusters grow in size. We find that exterior atoms have larger polarizabilities than interior atoms and that the charge transfer contribution to the total cluster polarizability increases with cluster size. We examine the relationship between the atomic polarizabilities in these clusters and bulk polarizability in carbon and silicon.

¹This work was supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, U. S. Department of Energy under grant number DE-FG02-03ER15489 (KAI, SS, and MY) under contract number DE-AC-02-06CH11357 (JJ).

2:03PM J26.00013 The Role of Vacancies on the Doping in Silicon Nanocrystals¹. JAE-HYEON EOM, TZU-LIANG CHAN, JAMES CHELIKOWSKY, University of Texas at Austin — We will present results for the effect of intrinsic defects (vacancies) on the doping of silicon nanocrystals by using first-principles calculations, i.e., pseudopotentials in real space. We calculated the total energy of a B doped silicon nanocrystal as a function of the vacancy position and the nanocrystal size. We found that the most stable B site strongly depends not only on the cluster size, but also on the position of the vacancy. We also explored the evolution of the interaction between the vacancy and the B dopant by comparing the total energy for several nanocrystal sizes and configurations.

¹This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

Tuesday, March 17, 2009 11:15AM - 1:51PM –
Session J27 GIMS: Focus Session: X-ray and Neutron Instruments and Sciences I 329

11:15AM J27.00001 Synchrotron X-ray Ultrafast Phase-Contrast Imaging Study of Fluids. YUJIE WANG, Argonne National Laboratory — Visible light imaging has been the traditionally dominant technique for study of fluid mechanical systems. However, it suffers from strong refraction, reflection and scattering effects under various occasions. X-ray phase-contrast imaging technique with its inherent generation synchrotron can offer a great tool for studying fluid mechanical systems with microsecond temporal and micron spatial resolutions. Several examples on dynamic multiphase flows and fluid singularities will be demonstrated. Future applications for other soft-condensed matter systems will also be discussed.

11:51AM J27.00002 Implicit spatial averaging in inversion of inelastic x-ray scattering data¹. P. ABBAMONTE², Frederick Seitz Materials Research Laboratory, University of Illinois — Inelastic x-ray scattering (IXS) is usually said to measure the imaginary part of the dynamical density response of a material. However this is not rigorously true. The density response χ, which describes the response of the system to a point charge source, is a function of two spatial coordinates and the time, i.e. χ = χ(x₁, x₂, t). Its Fourier transform χ(k₁, k₂, ω) is therefore a function of two, rather than just one, momenta. IXS does not probe this full response, but only its longitudinal or “diagonal” part Im{χ(k, k, ω)}. In this talk I will show that recently developed IXS inversion algorithms [2], which have shown promise for imaging attosecond dynamics in real space, yield a specific spatial average of the response, i.e. χ(x₁, t) = ∫ dx₂′ χ(x₁, x₂ + x₂′, t). This can be thought of as an average over all possible source locations, a real space projection, or a specific type of Fourier space filtering. I will show, within a simple model, that the salient real space dynamics nonetheless survive, and that IXS inversion is still a useful and well-posed technique for imaging attosecond dynamics.

¹This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

12:03PM J27.00003 Quasi-zero dimensional CuB₂O₄ as an archetype for resonant inelastic X-ray scattering. JASON HANOCO, GUILLAUME CHABOT-COUTURE, YUAN LI, Stanford, GUERMAN PETRAKOVSKI, Kirenski Institute, Siberia, KENJI ISHII, IGNACE JARRIGE, JUN-ICHIRO MIZUKI, JAEA, SPring8, MARTIN GRENEN, TOM DEVEREAUX, Stanford — We explore the general phenomenon of resonant inelastic scattering (RIXS) using CuB₂O₄, a network of CuO₂ plaquettes electronically isolated by B³⁺ ions. Spectra show a small number of well-separated features, and we exploit the simple electronic structure to explore RIXS phenomenology by developing a calculation allowing for intermediate-state effects ignored in standard approaches. These effects are found to be non-negligible and good correspondence between our model and experiment leads to a simple picture of such phenomenology as the genesis of d−d excitations at the K edge and intermediate-state interference effects.

12:15PM J27.00004 Inelastic Neutron Scattering Study of Ce₃Sn and Ce₃In. C.H. WANG, J. M. LAWRENCE, University of California, Irvine, CA. 92697 USA, A.D. CHRISTIANSON, Oak Ridge National Laboratory, Oak Ridge 37831, TN USA, E.A. GOREMYCHKIN, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom, E.D. BAUER, Los Alamos National Laboratory, Los Alamos, NM, 87545 USA, N.R. DE SOUZA, A.I. KOLESNIKOV, Argonne National Laboratory, Argonne, IL 60439 USA — In Ce₃Sn and Ce₃In, the linear coefficients of specific heat γ are 260 mJ/mol CeK² and 700 mJ/mol CeK², respectively. The Wilson ratio is 7.0 for Ce₃Sn and 11.5 for Ce₃In. Such large values suggest the presence of ferromagnetic correlations in the ground state. Hence, this system is a potential candidate for studying the magnetic instability at a quantum critical point (QCP). As an initial measurement, we have measured the magnetic inelastic neutron scattering line shape of polycrystalline samples to determine the crystal field (CF) excitations. The low temperature spectrum of both Ce₃Sn and Ce₃In consist of a quasi-elastic line and two obvious inelastic lines resulting from the two excited crystal field doublets of Ce⁺⁺ in the tetragonal symmetry. The quasi-elastic linewidth which is related to the Kondo scale, is 3.2mEV for Ce₃Sn and 1.5mEV for Ce₃In, consistent with the linear coefficients of specific heat. For Ce₃Sn the two CF excitations are at 20mEV and 35mEV while for Ce₃In, the splitting is much larger giving the two excitations at 15mEV and 47mEV.
12:27PM J27.00005 Resonant Multi-Wave X-Ray Diffraction Study on Iron Oxides System. SHIH-CHANG WENG, YEN-RU LEE, JHENG-GANG CHEN, CHIA-HUNG CHU, SHIH-LIN CHANG, National Tsing Hua University — The resonant X-ray scattering occurs when the incident photon energy is close to an absorption edge of a constituent atom. Under such circumstances, the corresponding atomic scattering factor will be modified due to anomalous dispersion, which is directly related to unoccupied states, magnetic moment, charge distribution, and the types of near-neighbor atoms. Therefore, the resonant X-ray scattering is widely used to investigate crystal structure, electronic structure, magnetic property and charge distribution, etc. On the other hand, the multi-wave diffraction can provide more information about reflection phase than the normal (two-beam) Bragg diffraction. In this paper, we will show that resonant multi-wave diffraction profiles in the vicinity of iron k-edge give the information about charge-ordering/charge distribution of iron oxide systems, such as Fe3O4.

12:39PM J27.00006 X-ray Diffuse Scattering from Ultrafast Laser Excited Solids. MARIANO TRIGO, YU-MIIN SHEU, JIAN CHEN, DAVID REIS, University of Michigan, STEPHEN FAHY, EAMONN MURRAY, University College, Cork, Ireland, TIMOTHY GRABER, ROBERT HENNING, University of Chicago — Intense, ultrashort laser pulses can be used to excite and detect coherent phonons in solids. However, optical experiments can only probe a reduced fraction of the Brillouin zone and hence most of the decay channels of such coherent phonons become invisible. In contrast, time-resolved x-ray diffuse scattering (TRXDS) has the potential to be the ultimate tool to study these phonon decay processes throughout the Brillouin-zone of the crystal. In our work, performed at the BioCARS beamline at the Advanced Photon Source, we use synchrotron time-resolved diffuse x-ray scattering to study Si and Bi under intense laser excitation with 100 ps resolution. We show that reasonable signal levels can be achieved with incident flux of $10^{12}$ photons comparable to the flux that will be available at future 4th generation sources such as the LCLS in a single pulse. These sources will also provide three orders of magnitude shorter pulses; thus, this experiment serves as a test of the feasibility of time-resolved X-ray diffuse scattering as a tool for studying nonequilibrium phonon dynamics in solids.

12:51PM J27.00007 Antiferromagnetism in a Fe50Pt40Rh10 thin film investigated using neutron diffraction1. GARY MANKEY, University of Alabama, DIETER LOTT, JOCHEN FENSKE, ANDREAS SCHREYER, GKSS Research Center, PRAKASH MANI, University of Alabama, FRANK KLOSE, Australian Nuclear Science and Technology Organization, WOLFGANG SCHMIDT, KARIN SCHMALZL, Juelich Research Center, ELENA TARTAKOVSKAYA, National Ukrainian Academy of Science — The temperature-dependent magnetic structure of a 200 nm thick single-crystalline film of Fe50Pt40Rh10 was studied by unpolarized and polarized neutron diffractions. By applying structure factor calculations, a detailed model of the magnetic unit cell was developed. In contrast to former studies on bulk samples, our experimental results show that the film remains in an antiferromagnetic state throughout the temperature range of 10–450 K. Remarkably, it can be demonstrated that the antiferromagnetic structure undergoes a smooth transition from a dominant out-of-plane order with the magnetic moments oriented in-plane to an in-plane order with the magnetic moments oriented perpendicular to the film plane. Theoretically, this can be explained by the existence of two competing anisotropy contributions with different temperature dependencies.

1 This work was supported by NSF and DOE/EPSCOR.

1:03PM J27.00008 Following Transient Phases at the Air/Water Interface1. MATI MERON, JEFF GEBHARTD, HAROLD BREWER, P. JAMES VICCARO, BINHUA LIN, CARS, The University of Chicago — A fast pixel array detector, the Pilatus 100K, has been used in studies of organic monolayers at the air-water interface. The area sensitivity and large dynamic range of the detector, in combination with a “one dimensional pinhole” geometry, make it possible to observe surface processes which were inaccessible to the previous generation of experimental techniques. Especially, time dependent phenomena acting on time scales ranging from seconds to minutes can be observed and analyzed.

1 This work is supported by ChemMatCARS, University of Chicago, which is funded by a NSF and DOE grant number CHE-0535644.

1:15PM J27.00009 Detecting Hidden Symmetries with Coherent X-Ray Diffraction1. THOMAS DEMMER, ALEJANDRO DIAZ ORTIZ, PETER WOCHNER, HELMUT DOSCH, Max Planck Institute for Metals Research — An approach to analyze x-ray coherent diffraction patterns of amorphous systems is presented. We have investigated archetype hard-sphere systems where the local environment is simulated using different hundreds of geometric structures (i.e., regular and irregular polyhedra). The effect of positional and orientation randomness on the coherent diffraction pattern is studied numerically for samples containing up to 107 particles. A library of such simulated diffraction data is then used to retrieve the underlying symmetries in amorphous systems. A discussion of the relevant experimental work is also presented.

1 This work has been funded by the Alexander von Humboldt Foundation

1:27PM J27.00010 Measuring phonon dispersion relations with momentum- and energy-resolved x-ray calorimetry. RUQING XU, U. of Illinois at Urbana-Champaign, HAWOONG HONG, Argonne National Lab, T.-C. CHIANG, UIUC — X-Ray Thermal Diffuse Scattering (TDS) is a powerful method for determining phonon dispersion relations, as has been demonstrated in a number of experiments. However, most previous studies employed a fitting procedure based on presumed atomic force constant models, and the results could be susceptible to systematic errors. In view of this issue, we have developed a new method based on momentum-resolved x-ray calorimetry. The phonon frequencies at specific wavevectors are determined directly from the temperature dependence of the TDS intensities, with no force constant models needed. A test of this method on Cu has yielded excellent results. However, a limitation exists for this method, as it requires data taken over a wide temperature range, and the minimum temperature must be significantly lower than the Debye temperature. This can be a problem for materials with phonon frequencies that change significantly with temperature. To overcome this problem, we are experimenting with another method: the scattered x-rays are energy analyzed, and the TDS intensity is determined relative to the Compton scattering intensity. With this internal intensity calibration, phonon frequencies can now be determined from TDS data with temperature. To overcome this problem, we are experimenting with another method: the scattered x-rays are energy analyzed, and the TDS intensity is determined relative to the Compton scattering intensity. With this internal intensity calibration, phonon frequencies can now be determined from TDS data over a narrow temperature range. Results of a test study on chromium will be presented.

1:39PM J27.00011 Infrared emission induced by x-rays1. RICHARD ROSENBERG, MOHAMMAD ABU HALA, Argonne National Laboratory, SIMON WATKINS, Simon Fraser University — Two of the most powerful methods for studying the properties of matter are Fourier transform infrared (FTIR) spectroscopy and synchrotron radiation (SR) based x-ray techniques. Having the ability to perform both types of research on the same samples at the same time would be a significant synergism. Furthermore, the spatial resolution of conventional FTIR microscopes is limited by diffraction, which in the mid IR is 2-20 μm, while SR based x-ray microscopes are capable of <30 nm diameter resolution. Thus, by utilizing nanometer sized x-ray beams to produce IR emission it should be possible to extend the spatial resolution of IR microscopy by orders of magnitude and simultaneously perform x-ray studies. To test the feasibility of this approach we have incorporated a commercial FTIR instrument into an existing ultra-high vacuum end station on an insertion device beamline at the Advanced Photon Source and measured the bandgap, exciton luminescence (0.4 eV) from InAs thin films. Results using both high intensity, near-zero-order and low intensity, monochromatic x-rays will be presented.

1 This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.
11:15AM J28.00001 Electronic properties of graphene and its operation at GHz frequencies
YU-MING LIN, IBM T. J. Watson Research Center — Graphene, a two-dimensional carbon crystal, possesses great potential for applications in nanoelectronics because of its high intrinsic carrier mobility and the possibility of being processed using the well-established planar top-down technology in semiconductor industries. The former makes graphene an ideal candidate for electronic devices operating at high frequencies, while the latter allows us to tailor the transport properties of graphene devices by controlling their channel geometry. For example, it is, in principle, possible to create metallic and/or semiconducting graphene nanostuctures if a precise edge termination can be achieved. In this talk, I will present our recent experimental studies on transport properties of graphene nanoribbons and high-frequence characteristics of graphene transistors operated at GHz frequencies. High-quality graphene nanoribbons with widths down to 30 nm are fabricated by e-beam lithography. In these graphene nanoribbon devices, clear plateau features are observed in the measured conductance as a function of gate voltage at T \( \lesssim 80 \) K, indicating the formation of subbands due to quantum confinement in nanoribbons. This conductance quantization behavior is observed in both metallic and semiconducting nanoribbons, and provides the direct experimental evidence of quantum size confinement effects and the formation of subbands for 1D graphene nanoribbons. To explore the high-frequency transport in graphene, top-gated graphene field-effect transistors are fabricated and S- parameter measurements are performed to obtain their transport properties at microwave frequencies. In these graphene transistors, we found that the measured intrinsic current gain shows the ideal 1/f frequency dependence, indicating an FET-like behavior in these devices. The cutoff frequency \( f_T \) at which the current gain becomes unity is proportional to the dc transconductance \( g_m \) of the device, and is consistent with the relation \( f_T = g_m/(2\pi C) \). The peak \( f_T \) was found to increase with a reducing gate length, and a cut-off frequency beyond 20GHz was measured in a graphene transistor with a gate length of 150 nm. This work is done in collaboration with Ph. Avouris, D. Farmer, K. Jenkins, A. Valdes-Garcia, V. Perebeinos, J. Small.

11:51AM J28.00002 Graphene Frequency Multipliers1. HAN WANG, DANIEL NEZICH, JING KONG, TOMAS PALACIOS, Massachusetts Institute of Technology — In this paper we demonstrate a new application for graphene: full-wave signal rectification and frequency doubling. Due to its ambipolar transport properties, graphene field-effect transistors (GFET) show a V-shaped transfer characteristic about the minimum conduction point. Frequency doubling can be realized with a single GFET by biased the gate to the minimum conduction point and superimposing a sinusoidal input signal to the gate. Electrons and holes will conduct in alternative half cycles to produce an output signal at the drain, whose fundamental frequency is twice that of the input. Sub-linear IV characteristics of the GFET near minimum conduction point help improve the conversion efficiency and spectrum purity of the output signal. In our experiments, for an input frequency of 10 KHz, the output signal showed excellent spectrum purity (94% of RF power at 20 KHz) in the absence of any filtering elements. Given the extremely high electron mobility in graphene (>100,000 cm^2/Vs at room-temperature), such ambipolar devices have the potential to operate at very high frequencies and allow the fabrication of new THZ sources and sensors, as well as high speed transmitters and receivers.

1This work is partially supported by Interconnect Focus Center (IFC) and Microsystems Technology Laboratories MIT.

12:03PM J28.00003 Chemically derived graphene nanoribbons: physical properties and electronics1, XINRAN WANG, Stanford University, YIJIAN OUYANG, University of Florida, XIAOLIN LI, LI ZHANG, HAILIANG WANG, Stanford University, JING GUO, University of Florida, HONGJIE DAI, Stanford University — Graphene electronics is a promising field of graphene research due to extremely high carrier mobility and the ability to fabricate true nanometer scale devices. We show that sub-10nm graphene nanoribbons, which are semiconductors with suitable bandgap for nanoelectronics, can be synthesized via chemical methods. Electrical transport measurements show that GNRs have finite bandgaps which are inversely proportional to widths. Unlike carbon nanotubes, all the sub-10nm GNRs are semiconductors and afford graphene field-effect transistors (FETs) with on-off ratio higher than 10^6 at room temperature. The performance of individual GNRFET is assessed and compared with CNTFETs. The scattering free path of carriers in GNRs is estimated, and the limiting factors are discussed. The performance of chemical GNRs and plasma etched GNRs are also compared and discussed.

1This work was supported by Intel, MARCO MSD and ONR.

12:15PM J28.00004 Non-volatile memory devices using graphene and ferroelectric thin films1, YI ZHENG, National University of Singapore — The unique linear energy band dispersion and its purely 2D crystalline structure have made graphene a rising star not only for fundamental research but also for nanoscale device applications. Here we demonstrate a novel non-volatile memory device using a combination of graphene and a ferroelectric thin film. The binary information, i.e., “1” and “0”, is represented by the high and low resistance states of the graphene working channels and is switched by the polarization directions of the ferroelectric thin film. A highly reproducible resistance change exceeding 300% is achieved in our graphene-ferroelectric hybrid devices under ambient conditions. The experimental observations are explained by the electrostatic doping of graphene by the remnant electrical field at the ferroelectric/graphene interface.

1In collaboration with Dr. Kui Yao, Institute of Material Research and Engineering, Singapore, and Dr. Barbara Oezylmar, National University of Singapore.

12:51PM J28.00005 Tuning Disorder and Interactions in Graphene1. JIANHAO CHEN, Department of Physics, University of Maryland — One (of many) unique aspects of graphene is that it is an atomically-thin two-dimensional electron system, open to manipulation and study using surface science techniques. This aspect of graphene has allowed us to tune both the disorder strength the interaction strength, allowing unprecedented control over a condensed matter system. Experiments are performed on atomically-clean graphene on SiO\(_2\) in ultra-high vacuum. Addition of potassium to graphene is used to study the dependence of the mobility and minimum conductivity point on charged impurity density. Tuning the dielectric environment through addition of an ice overlayer has two effects: charged impurity scattering is reduced, due to reduced Coulomb interaction between impurities and carriers, while short-range scattering is increased, due to reduced screening. In sharp contrast to graphene with charged impurity disorder, which remains metallic at low temperature, even a small amount of irradiation-induced point disorder produces a divergence of the resistivity and insulating behavior at low temperature.

1Supported by the NSF Maryland MRSEC, Nanoelectronics Research Institute, and Office of Naval Research.

1:27PM J28.00006 Graphene electronics: joule heat and charge density in active devices. MARCUS FREITAG, MATHIAS STEINER, YVES MARTIN, VASILI PEREBEINOS, ZHIHONG CHEN, JAMÉS C. TSANG, PHAEDON AVOURIS, IBM TJ Watson Research Center — We use Raman scattering microscopy to measure the shifts of the 2D and G-bands resulting from the electronic power dissipation in the graphene sheet. Extracted images of the temperature distribution show peak temperatures of up to 1000K in the middle of the graphene device. The metallic contacts act as the dominant heat sinks, because the thermal conductivity of graphene is far greater than the gate-oxide thermal conductivity. We model thermal transport and obtain excellent agreement in peak temperature and functional form. Velocity saturation due to phonons with 50meV energy is observed, suggesting that substrate polar phonons limit the high-bias conduction in graphene. Trapped charges are also detected and we find that application of a high current is associated with drain-induced barrier lowering in back-gated graphene devices.
1:39PM J28.00007 n-Type Behavior of Graphene Supported on Si/SiO2 Substrates1, HUMBERTO GUTIERREZ, HUGO ROMERO, NING SHENG, JORGE SOFO, PETER EKLUND, Physics Department, Penn State University, PARSOON JÔSHI, SRINIVAS TADIGADAPA, Electrical Engineering Department, Penn State University — Results are presented from an experimental and theoretical study of electronic properties of back-gated graphene field effect transistors (FETs) on Si/SiO2 substrates. The excess charge on the graphene was observed by sweeping the gate voltage to determine the charge neutrality point in the transistors. Devices exposed to laboratory environment for several days were always found to be initially p-type. After \( \sim 20 \) h at 200 °C in \( \sim 5 \times 10^{-7} \) Torr vacuum, the FET slowly evolved to n-type behavior with a final excess electron density on the graphene of \( 4 \times 10^{12} \) electrons/cm\(^2\). This value is in excellent agreement with our theoretical calculations on SiO\(_2\), where we have used molecular dynamics to build the SiO\(_2\) and then density functional theory to compute the electronic structure. The essential theoretical result is that SiO\(_2\) has a significant surface state density just below the conduction band edge that donates electrons to the graphene to balance the chemical potential at the interface. An electrostatic model for the FET is also presented that produces an expression for the gate bias dependence of the carrier density.

3This work is supported by NSF NIRT ECS 06-09243.

1:51PM J28.00008 Photocurrent imaging and efficient photon detection in a graphene transistor1, FENGNIAN XIA, THOMAS MUELLER, IBM TJ Watson Research, ROKSANA GOLIZADEH-MOJARAD, ECE Department, Purdue University, MARCUS FREITAG, YU-MING LIN, JAMES TSANG, VASILI PEREBEINOS, PHAEDON AVOURIS, IBM TJ Watson Research — We measure the channel potential of a graphene transistor using a scanning photocurrent imaging technique. In this approach, the photon-induced current between the source and drain is measured when the excitation laser beam is scanned across device at various gate biases. Potential profiles are then inferred from photocurrent measurements. We show that at a certain gate bias, the impact of the metal on the channel potential profile extends into the channel for more than 1/3 of the total channel length from both source and drain sides, hence most of the channel is affected by the metal. The barrier height between the metal and graphene interface is experimentally determined to be around 95 meV from transport and photocurrent measurements. As the gate bias exceeds the Dirac point voltage, \( V_{\text{Dirac}} \), the original p-type graphene channel turns into a p-p-n channel. When laser beam from He-Ne laser with a wavelength of 632.8 nm is focused on the p-n junctions, an impressive external responsivity of \( \sim 0.001 \) A/W is achieved, given that only a single layer of atoms are involved in photon detection. The possibility of using graphene p-n junctions in high-bandwidth photonic applications is discussed.

2:03PM J28.00009 Quantum capacitance measurement in high performance graphene field-effect devices1, ZHIHONG CHEN, IBM T.J. Watson, JOERG APPENZELLER, Electrical Engineering, Purdue University — We demonstrate first quantum capacitance measurements on single-layer graphene devices and elucidate on their relevance for the extraction of mobility for scaled graphene FETs. We also show experimentally that multi-layer graphene devices can be easily distinguished from single-layer graphene within our capacitance measurement approach, a previously unnoticed fact.

Tuesday, March 17, 2009 11:15AM - 2:15PM –
Session J29 GMG DMP FIAP: Focus Session: Spin Currents in Metals - New and Miscellaneous Topics 333

11:15AM J29.00001 Electronic transport in ferromagnetic conductors1, CHRISTIAN WICKLES, WOLFGANG BELZIG, University of Constance — We theoretically study ferromagnetic conductors using the Stoner model to describe the interaction between electron spin and magnetization. The latter can, in general, depend on time and space. We include impurity scattering processes for the electrons that lead to momentum relaxation, spin-flip and spin-dephasing. Utilizing Keldysh theory, we derive transport equations which allow to access interesting quantities such as domain wall resistance, electronic contribution to the magnetization damping coefficients and forces induced by non-equilibrium electron distributions in the presence of current flow. On the other side, a magnetization that shows temporal and spatial variation can induce current flow in the electron system.

11:27AM J29.00002 Bulk Spin Pumping and Bulk Spin Transfer Torque in Two-band Magnetic Conductors1, WAYNE SASLOW, Texas A&M University — For nonmagnetic materials, irreversible thermodynamics shows that thermal conduction and electrical conduction have a new and independent cross-coupling that yields a thermoelectric and an electrothermal effect. All of these terms are dissipative. However, for nonuniform two-band conducting magnets (e.g., within domain walls), electrical conduction and magnetization dynamics are cross-coupled by the up-band and down-band conductivities, without a need for a new cross-coupling. This yields both a bulk spin pumping term driving the current and a bulk spin transfer torque term driving the magnetization. Adiabatic in space, these terms are dissipative. In addition to these spin transfer and spin pumping terms corresponding to existing transport coefficients, for each spin component there are two types of additional transport coefficients. One type modifies the dissipative conductivity-driven terms in spin pumping and spin transfer torque, and itself is dissipative. The other type, non-adiabatic in space, is non-dissipative. We consider the situation where there is a spin current but no net current. Thermal effects are also considered, with temperature gradients having the same symmetry as gradients in the up and down spin electrochemical potentials.

2This work supported by the DOE through grant #DE-FG02-06ER46278.

11:39AM J29.00003 Influence of a Transport Current on Magnetic Anisotropy1, ION GARATE, ALLAN MACDONALD, University of Texas at Austin — The microscopic understanding of the spin transfer torque (STT) is an essential ingredient in the quest to develop optimized spintronic devices. It is well-known that STT occurs whenever electric currents travel through non-collinear magnetic systems. In contrast, it is often overlooked that current-induced torques may also arise in uniformly magnetized systems due to the intrinsic spin-orbit coupling in the band structure of the ferromagnet. We relate this effect to the change in magnetic anisotropy in presence of a current, and use simple models to estimate the possible role of transport currents to modify the direction of the ferromagnetic easy axis and assist magnetization reversal.

11:51AM J29.00004 Quantifying Spin Hall Effects in Gold Hall Bars1, GORAN MIHAJLOVIC, JOHN E. PEARSON, SAMUEL D. BADER, AXEL HOFFMANN, Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439 USA, MIGUEL ANGEL GARCIA, Universidad Complutense, Madrid, Spain — Spin Hall effects manifest the fundamental interdependence between charge and spin transport. We studied these effects experimentally by measuring the non-local resistance, \( R_{nl} \), in mesoscopic Au Hall bars where spin current generation and detection are spatially separated in two side arms, while a bridging arm acts as the spin conduit. The measured \( R_{nl} \) decreases monotonically with decreasing temperature, changing sign from positive to negative. This can be understood by modeling \( R_{nl} \) as a sum of two components: a positive, ohmic component, arising from the charge current, and a negative component, due to spin Hall effects and spin diffusion. By varying the spacing between the side arms, the components can be separated. We determined the spin diffusion length, thespin Hall angle and the spin Hall conductivity. We found spin Hall angles of order 0.1, with a temperature dependence proportional to the resistivity, while the spin Hall conductivity was almost temperature independent.

3Work at Argonne is supported by the U.S. Department of Energy Office of Science under Contract No. DE-AC02-06CH11357.
12:03PM J29.00005 Investigation of Spin-Torque Effects on the Exchange Bias of Ferromagnet/Antiferromagnet Bilayers, KIRAN V. THADANI, R.A. BUHRMAN, D.C. RALPH, Cornell University — Spin-polarized current, generated by one ferromagnetic layer in a magnetic multilayer structure, can deposit spin angular momentum into a second ferromagnetic layer, causing it to either reversibly switch its orientation or oscillate in steady state at microwave frequencies. Recent calculations and experiments have investigated the possibility that spin torque might also alter the structure of an antiferromagnet [1], thereby affecting the exchange-bias field produced by the antiferromagnet on an adjacent ferromagnetic layer [2, 3]. Here we report studies made using nanopillar samples in which the free magnetic layer is exchange-biased to an antiferromagnet, which allow a direct measurement of the magnitude of the exchange bias and its current dependence. We will also investigate the degree to which the exchange bias alters the damping of the free-layer magnet and the extent to which the effective damping can be controlled with current. [1] A. S. Nunez et al., Phys. Rev. B 73, 214426 (2006). [2] Z. Wei et al., Phys. Rev. Lett. 98, 116603 (2007). [3] S. Urazhdin et al., Phys. Rev. Lett. 99, 046602 (2007).

12:15PM J29.00006 Tunnel barrier enhanced voltage signals generated by magnetization precession of a single ferromagnetic layer¹, TAKAHIRO MORIYAMA, University of Delaware — A variety of experimentally observed phenomena involving nonlocal magnetization dynamics in magnetic multilayers are due to two complementary effects: (i) the transfer of spin angular momentum accompanying charge currents driven by the applied bias voltage between ferromagnetic layers results in torques that (for sufficiently high current densities) generate spontaneous magnetization precession and switching; and (ii) the precessing magnetization of a ferromagnet (FM) pumps spins into adjacent normal metal layers (NM) with no applied bias. In particular, the spin pumping effect is a promising candidate for realizing a spin battery device [1] as a source of elusive pure spin currents (not accompanied by any net charge transport) emitted at the FM/NM interface, where steady magnetization precession of the FM layer is sustained by the absorption of external rf radiation under the FMR conditions. We report the electrical detection of magnetization dynamics in an Al/AI0₂/Ni₈₀Fe₂₀/Cu tunnel junction, where a Ni₈₀Fe₂₀ ferromagnetic layer is brought into precession under the ferromagnetic resonance (FMR) conditions. The dc voltage generated across the junction by the precessing ferromagnet is enhanced about an order of magnitude compared to the voltage signal observed in Cu/FeNi/Pt structures [2]. A structure of Cu (100nm)/Al (10nm)/AlOₓ (2.3nm)/Ni₈₀Fe₂₀ (20nm)/Cu (70nm)/Au (25nm) was fabricated on a Si substrate with a 1µm thick thermal oxide layer. The bottom-most 100 nm Cu layer was patterned into a coplanar waveguide (CPW) and the rest of the structure was patterned into a pillar structure on the signal line of the CPW. Dc voltages ~ µV were observed in the Al/AlO₂/Ni₈₀Fe₂₀/Cu tunnel junction when the Ni₈₀Fe₂₀ is in the ferromagnetic resonance. The dc voltages increase as the precession cone angle and frequency increase. We discuss the relation of this phenomenon to magnetic spin pumping and speculate on other possible underlying mechanisms responsible for the enhanced electrical signal. [1] A. Brataas et al. PRB 66, 060404 (2002) [2] M. V. Costache et al. PRL 97, 216603 (2006)

¹This work was supported by NSF DMR Grant No. 0405136, and DOE DE-FG02-07ER46374

12:51PM J29.00007 FMR and voltage induced transport in normal metal-ferromagnet-superconductor trilayers, HANS JOAKIM SKADSEEM, ARNE BRATAAS, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway, JAN MARTINEK, Institute of Molecular Physics, Polish Academy of Science, 60-179 Poznan, Poland — In recent years, hybrid nanoscale circuits containing normal conductors, ferromagnets, and superconductors have been realized. These structures allow observation and understanding of the competition between ferromagnetism and superconductivity. In this talk, we consider charge and spin transport in normal metal-ferromagnet-superconductor trilayers induced by bias voltage and/or magnetization precession. Transport properties are discussed in terms of time-dependent scattering theory. We compute the charge and spin current response to bilinear order in precession frequency and bias voltage and express the results in terms of spin-dependent conductances. Simplified conductance expressions are obtained when the ferromagnet is longer than the transverse spin coherence length.

1:03PM J29.00008 Spin torque from tunneling through impurities in a magnetic tunnel junction, TURAN BIROL, PIET BROUWER, Cornell University — We study impurity-mediated transport in a magnetic tunnel junction (MTJ) in the sequential tunneling regime. We address the conductance of the MTJ as well as the spin transfer torque. We show that the torque from impurity-mediated tunneling can be distinguished from that from direct tunneling through its dependence on the barrier thickness and the angle between the ferromagnetic moments.

1:15PM J29.00009 Thermoelectric transport and thermal spin currents in ferromagnetic films and nanostructures, AZURE AVERY, RUBINA SULTAN, BARRY ZINK, University of Denver — For fundamental physics, understanding the mechanisms behind giant magnetoresistance (GMR) and its related properties, magnetoresistance (MR) and magnetothermopower (MTEP), is crucial, especially for nanoscaled structures. Though progress has been made in understanding electron transport through magnetic thin films and multilayers, far less is understood about the mechanisms behind thermal transport in these systems. This is due, in part, to the difficulty of measuring thermal properties of these low-dimensional systems. We present a robust technique for accurately measuring thermal conductivity (kₜ), thermopower (α), and MTEP in nanoscale magnetic materials using micromachined silicon nitride thermal isolation structures. We outline the fabrication of the structures and present our measurement results for ferromagnetic thin films and nanowires. Finally, we present how this technique is applied to testing the validity of current models explaining the mechanisms of thermal transport, such as thermal spin currents, in ferromagnetic films and nanostructures.

1:27PM J29.00010 ABSTRACT WITHDRAWN —

1:39PM J29.00011 Magneto resistive junctions based on epitaxial graphene and h-BN, OLEG YAZYEV, ALFREDO PASQUARELLO, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — Using a first-principles approach, we investigate the structural, magnetic and transport properties of interfaces based on epitaxially grown monolayer graphene and hexagonal boron nitride (h-BN) in combination with ferromagnetic transition metals (Fe, Co and Ni). Such structurally well defined interfaces based on (111) fcc or (0001) hcp transition metal thin films can be produced using simple manufacturing processes. Our calculations predict magnetoresistance ratios over 100% for certain junction compositions. In addition, such systems feature strong antiparallel (Fe and Co) and parallel (Ni) exchange coupling across the interface combined with low junction resistance. The predicted properties position such magneto resistive junctions as an interesting alternative to the currently used giant and tunneling magnetoresistive systems and make them suitable for practical applications.
and this in turn produces coupling to the electric dipole moments. The oxygen distortions induced with the spin reorientations below $T_N$ distorts the MnO$_5$N in the Lu-O bonds. This suggests an enhancement of the net electric polarization below $T_N$ hereby show that it is the ferroelectric motion of the Lu ions coupled with O distortions that exhibits a strong temperature dependence below $T_N$. While in previously reported neutron diffraction data, it was shown that all atomic coordinates changed based on symmetry considerations with $T_N$, the multiferroic LuMnO$_3$ give systems such as YING ZOU, SHISHIR RAY, SOMADITYA SEN, MARK WILLIAMSEN, Dept of Physics, University of Wisconsin-Milwaukee, USA — Unconventional magnetic switching, in spin based electronics, and as materials with negative refractive index, make them important candidates for device applications. Here we present Rietveld and XAFS analysis will be made. The detailed temperature dependent structure on multiple length scales will be presented with implications for the method based on high-q data. Temperature dependent measurements reveal anomalies in the short range structure involving oxygen atoms. Comparison with Rietveld and XAFS analysis will be made.

Acknowledgements: NSF, UWM RGI, NASA, AAF

2:03PM J30.00003 Magnetic Field Dependent Changes in the Local Structure of ReMn$_2$O$_5$. M. DELEON, T.A. TYSON, Z. CHEN, NJIT, S.-W. CHEONG, Rutgers University — The temperature dependent structure of the ReMn$_2$O$_5$ (Re=rare earth) system has been examined by the x-ray pair distribution function method based on high-q data. Temperature dependent measurements reveal anomalies in the short range structure involving oxygen atoms. Comparison with Rietveld and XAFS analysis will be made. The detailed temperature dependent structure on multiple length scales will be presented with implications for the observed low temperature ferroelectric properties. This work is supported by DOE Grant DE-FG02-07ER46402.

12:15PM J30.00004 Studies of Competing Order in Multiferroic RMnO$_3$. PRASENJIT GUPTASARMA, YING ZOU, SHISHIR RAY, SOMADITYA SEN, MARK WILLIAMSEN, Dept of Physics, University of Wisconsin-Milwaukee, USA — Unconventional magnetic order, a ferroelectric background and the possibility of coupled ground states, together with competing spin, charge, lattice and orbital degrees of freedom, give systems such as RMnO$_3$ (R=Rare Earth), an ABO$_3$-type compound, a rich and fascinating phenomenology. The possibility of using these materials in switching, in spin based electronics, and as materials with negative refractive index, make them important candidates for device applications. Here we present a review of our studies of the detailed phenomenology of a series of single crystals of RMnO$_3$ grown from a floating zone, for different Rare Earths $R$, and by inducing structural distortions and charge disproportionation through substitutions at both the A and the B sites.

2:27PM J30.00005 Enhanced local lattice distortions with the antiferromagnetic transition in the multiferroic LuMnO$_3$. DESPINA LOUCA, University of Virginia, THOMAS PROFFEN, Los Alamos National Laboratory, SEUNG-HUN LEE, University of Virginia, SANG-WOOK CHEONG, Rutgers University — The ferroelectric hexagonal manganite, LuMnO$_3$, has been investigated via neutron scattering and the pair density function analysis to determine the nature of the local atomic distortions with the antiferromagnetic transition, $T_N$, of the Mn ions. While in previously reported neutron diffraction data, it was shown that all atomic coordinates changed based on symmetry considerations with $T_N$, we hereby show that it is the ferroelectric motion of the Lu ions coupled with O distortions that exhibits a strong temperature dependence below $T_N$ as reflected in the Lu-O bonds. This suggests an enhancement of the net electric polarization below $T_N$. At the same time, the motion of the apical O1 and O2 ions distorts the MnO$_5$ bipyramids, leading to more buckling of the ab-layers. However, the Mn ions do not appear to distort significantly away from their equilibrium position. The oxygen distortions induced with the spin reorientations below $T_N$ may be the cause for the Lu ion displacements through electrostatic interactions and this in turn produces coupling to the electric dipole moments.
Laboratory, Carnegie Institution of Washington, JINZHU HU, X17 of NSLS, CARS, University of Chicago, Upton, NY, CHENGLIN ZHANG, SUNG-BAEK KIM, R MnO.

In order to induce multiferroic behaviour in other magnetic members of the orthorhombic $R_{3d}$, and Ho 5d and Y 4d spectral features, the corresponding features in the Y

The effect of hydrostatic pressure on the ferroelectric properties of these systems will be given based on comparisons with density functional calculations.

12:39PM J30.00006 Pressure Dependence of Structure Stability of Multiferroic Hexagonal-RMnO$_3$, ZHIQIANG CHEN, PENG GAO, TREvor A. TYSOn, Department of Physics, New Jersey Institute of Technology, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, JINZHU HU, X17 of NSLS, CARS, University of Chicago, Upton, NY, CHENGLIN ZHANG, SUNG-BAEK KIM, SANG-WOOK CHEONG, Dept. of Physics and Astronomy, Rutgers University — We present high pressure IR and X-ray diffraction measurements of the hexagonal multiferroic systems HoMnO$_3$, YMnO$_3$ and LuMnO$_3$. Measurements were conducted over the pressure range ambient to $\sim$20 GPa. No phase changes were observed over this broad range of hydrostatic pressures. These suggest that the hexagonal structure is stable at higher pressures. The thermal treatment is necessary to overcome the barrier (breaking and reconnection of bonds) to achieve the hexagonal to orthorhombic phase change. A discussion of the effect of hydrostatic pressure on the ferroelectric properties of these systems will be given based on comparisons with density functional calculations.

This work is supported by DOE grant DE-FG02-07ER46402.

12:51PM J30.00007 X-ray absorption spectroscopy studies of YMnO$_3$, HoMnO$_3$, and Y$_3$Ho$_{0.5}$MnO$_{1.5}$, RELJA VASIC, North Carolina State University, DARIO ARENA, JOSEPH DVORAk, Brookhaven National Laboratory, HAILDong ZHOU, CHRIS R. WIEBE, National High Magnetic Field Laboratory, GERALD LUCOVSKY, North Carolina State University, MARC ULRICH, Army Research Office — We have investigated three hexagonal perovskites, YMnO$_3$, HoMnO$_3$, and Y$_3$Ho$_{0.5}$MnO$_{1.5}$ by O K$\alpha$ and Mn L$_{3,2}$ edge X-ray absorption spectroscopy. In YMnO$_3$ and HoMnO$_3$ the lowest energy transitions are predominantly Mnp 4p and 3d states with a least five distinct states occurring at approximately the same X-ray energies in both samples. We associate this portion of electronic structure with the trigonal bipyramidal bonding symmetry of a five-fold coordinated Mn. Higher energy transitions in the XAS OK$\alpha$ spectra are broader and associated with Ho 5d and Y 4d orbitals. Compared with YMnO$_3$ and HoMnO$_3$ Mn 3d, and Ho 5d and Y 4d spectral features, the corresponding features in the Y$_3$Ho$_{0.5}$MnO$_{1.5}$ K$\alpha$ spectrum exhibit broader features fewer in number. These are consistent with random alloy bonding in which the Ho and Y are randomly distributed on the A-atom sub-lattice. We will discuss the electronic structure of these empty states in the context of symmetry adapted linear combinations of molecular orbital O 2p*, and Mn 3d*, Ho 5d* and Y 4d* nearest neighbor states.

1:03PM J30.00008 Competing Magnetic Interactions in Magnetoelectric YbMnO$_3$, SHISHIR RAY, YING ZOU, MARK WILLIAMSEN, SOMADITYA SEN, LARRY BUROKER, PRASENJIT GUPTASARMA, Physics Dept, University of Wisconsin-Milwaukee, USA — The (RE)MnO$_3$ (RE = Rare Earth) series of magnetoelectrics exist as both hexagonal and orthorhombic lattice structures. These have recently attracted much attention due to possible applications in spintronics, in switching, and as media with negative refractive index. YbMnO$_3$ is hexagonal with ferroelectricity (Tc $\sim$ 970K) and antiferromagnetism (T N $\sim$ 80K). Comprehensive resonant X-ray scattering at variable temperatures (200-1000K) in a single crystal of magnetoelectric orthorhombic TbMnO$_3$ has been extensively studied both experimentally and theoretically about its fascinating properties (e.g., magneto-electric coupling, spiral magnetic order). Understanding these empty states in the context of symmetry adapted linear combinations of molecular orbital O 2p*, and Mn 3d*, Ho 5d* and Y 4d* nearest neighbor states.

Detailed description will be dealt with this presentation.

3:39PM J30.00011 Emergence of the multiferroic state in R$\text{MnO}_3$, G. BALAKRISHNAN, D. O'FLYNN, C.V. TOMY, M.R. LEES, Department of Physics, University of Warwick, Coventry CV4 7AL, UK — In order to understand the emergence of multiferroic behaviour in the R$\text{MnO}_3$ compounds, it is educational to study the relationship between ferroelectricity and magnetoelectrically enhanced lattice modulations in $\text{R MnO}_3$. Lattice modulations in $\text{R MnO}_3$ are strongly dependent on the Mn-O-Mn bond angle (\(\phi\)), which in turn is determined by the ionic radii (\(r_{\text{i}}\)) of the R atoms. Multiferroic properties have been observed in the orthorhombic R$\text{MnO}_3$ (R = Tb/Dy) compounds, in which \(\phi\) is close to 145°. In order to induce multiferroic behaviour in other magnetic members of the orthorhombic R$\text{MnO}_3$, and to tune the structure to be in the same region of the phase diagram as Tb/DyMnO$_3$, it is necessary to substitute at the R site with a suitable (smaller) atom. We have achieved this in SmMnO$_3$ and NdMnO$_3$ by substitutions at the Sm and Nd sites with smaller R ions. In the optimally substituted compounds (40 to 50%), we observe an additional magnetic transition. Investigations of the dielectric properties of the crystals reveal anomalies in the dielectric properties coincident with this magnetic transition, analogous to those exhibited by Tb/DyMnO$_3$, indicative of multiferroic behaviour. We present detailed investigations of the magnetic, dielectric and structural properties in single crystals of selected compositions.
11:15AM J31.00001 400-Fold Reduction in Saturation Field by Stress Relief in Multilayers. WILLIAM EGGLEHOF, JOHN BONEVICH, CARLOS BEAUCHAMP, GERY STAFFORD, JOHN UNGURIS, NIST, PHILIP PONG, University of Hong Kong, ROBERT EICMAEL, NIST — A common problem in soft magnetic thin films is increased saturation field due to stress build-up with increasing thickness. We have found a solution to the problem using multilayers of a magnetic thin film and a film that is either not lattice matched or has a different crystal structure. Reductions in the saturation field as large as 400 fold are found. The ultra-soft Ni$_2$Fe$_{14}$Cu$_8$Mo$_4$ alloy can have saturation fields as small as 0.05 mT (0.05 Os) for 10 nm thick films. However, for films 400 nm thick (which is needed for some applications) the saturation field is typically 20 mT. Splitting this magnetic thin film up into segments 100 nm thick separated by a 5 nm Ag film reduces the saturation field to 0.05 mT. Alternatively, using a 2 nm CoFe film yields a saturation field of 0.1 mT. A tensile stress of $7.35 \times 10^7$ dynes/cm$^2$ was measured in the 400 nm film and $3.7 \times 10^7$ dynes/cm$^2$ for the multilayer with Ag. The highly-stressed Ni$_2$Fe$_{14}$Cu$_8$Mo$_4$ develops a magnetostriction coefficient of $-5$ ppm, although in the unstressed state its magnetostriction coefficient is near zero. In conclusion, we have found a solution to the stress-induced large saturation fields in an otherwise soft magnetic film. The results should be important for ultra-low-magnetic-field tunnel-junction sensors and magnetic flux concentrators.

11:27AM J31.00002 Structure and magnetic properties of magnetron-sputtered FePt/Au superlattice films. YONGSHENG YU, University of Nebraska, HAIBO LI, Jilin Normal University, XINGZHONG LI, LANPING YUE, University of Nebraska, WEILI LI, Habbin Institute of Technology, MEI LIU, YUMEI ZHANG, Jilin Normal University, WEIDONG FEI, Habbin Institute of Technology, DAVID J. SELLMYER, University of Nebraska — FePt/Au multilayer films were prepared with sputtering and the effects of Au thickness and annealing temperature on the structure and magnetic properties were investigated. Superlattice structure was induced by thicker Au layer. The interatomic spacing d(220) in the fcc FePt lattice increases with increasing Au thickness, indicating increasing strain energy in fcc FePt lattice. After annealing at 300°C, FePt films with Au layer of 3.5 nm became ordered and the multilayer structure was retained. The strain energy in fcc FePt lattice appears to be responsible for lowering the ordering temperature of the FePt phase. For films annealed at higher temperatures, thicker Au layer restrained the ordering of FePt phase, which led to a decrease of coercivities. — This research is supported by DOE and NCMN.

11:39AM J31.00003 Controlling Interlayer exchange coupling in ultra narrow Fe/Pt multilayered nanowire: an ab initio study. PUSPAMITRA PANIGRAHI, RANJIT PATI, Michigan Technological University, Houghton, MI 49931 — Interest in the study of magnetic/non-magnetic multilayered structures took a giant leap since Grünberg and his group established that the value of interlayer exchange coupling (IEC) depends upon the non-magnetic spacer width. The recent increase in demand for device miniaturization compelled researchers to look for novel nanoscale multilayered structures. Towards this effort, we have studied IEC in one dimensional Fe/Pt multilayered nanowires using first principles density functional approach. Our result shows the exchange coupling energy (J) to switch sign as the width of the non-magnetic Pt spacer varies. The competition among short and long range direct exchange and the super exchange is recognized to play an important role for the non-monotonic sign of IEC depending upon the width of the Platinum spacer layer.

11:51AM J31.00004 Design of Co/Pd multilayer system with antiferromagnetic-to-ferromagnetic phase transition. JAN-ULRICH THIELE, Seagate Technology — Among the known magnetic material systems there are only very few examples of materials that undergo a temperature dependent antiferromagnetic-to-ferromagnetic phase transition, and of these only the chemically ordered alloy FeRh exhibits this transition near room temperature [1, 2]. Here we present a perpendicular anisotropy multilayer structure that mimics FeRh. The basic idea is to use two stacks of Co/Pd multilayers with large perpendicular magnetic anisotropy and high Curie temperature, $T_C$, separated by a layer providing antiferromagnetic coupling, and a CoNi/Pd multilayer with perpendicular anisotropy with a lower $T_C$, interlayer, in the range of the desired AF-FM transition temperature, $T_{AF-FM}$. At room temperature this system behaves as two antiferromagnetically coupled layers with a low perpendicular remanent magnetic moment. As the temperature is raised to approach $T_{C,interlayer}$ the magnetization of the interlayer is gradually reduced to zero, and consequently its coupling strength is reduced. Eventually, the effective coupling between the two high-$K_{c,interlayer}$, high-$T_C$ layers becomes dominated by their dipolar fields, resulting in a parallel alignment of their moments and a net remanent magnetic moment equal to the sum of the moments of the two high-$T_C$ layers [2].


12:27PM J31.00005 Graded Magnetic Anisotropy in Co/Pd Multilayers. B. J. KIRBY, J. E. DAVIES, National Institute of Standards and Technology, S. M. WATSON, R. D. SHULL, J. A. BORCHERS, National Institute of Standards and Technology, G. T. ZIMANYI, KAI LIU, University of California - Davis — As the magnetic recording industry looks beyond perpendicular recording, multilayered exchange coupled media have demonstrated potential for increased storage density. Recent work has shown further enhancements when the anisotropy is gradually increased from a soft top to a hard bottom region. However, creating graded anisotropy structures is difficult, and convincingly demonstrating such a gradient is also challenging. Since the coercivity of Co decreases with increasing thickness, we attempted to create graded anisotropy structures by sputtering Co/Pd superlattices with progressively varying Co layer thicknesses. We probed the depth dependent anisotropy of the samples using polarized neutron reflectometry (PNR), a technique sensitive to the depth-dependent magnetic composition of thin films. The sample magnetization vector M was bent away from the out-of-plane easy axis direction by an applied magnetic field H, and the depth profile of the in-plane component of M(H) was measured. Our results clearly demonstrate that samples with graded Co thickness also exhibit graded anisotropy. Further, comparisons of samples with different levels of gradient discretization shed light on the nature of the interlayer exchange coupling in a graded anisotropy system. [1] D. Suess, Appl. Phys. Lett. 89, 189901 (2006).

12:39PM J31.00006 Coercivity enhancement in (Co/CoO)$_n$ superlattices. SRINIVAS POLISSETTY, CHRISTIAN BINEK, University of Nebraska-Lincoln — The temperature dependence of the coercivity is studied in (Co/CoO)$_n$ periodic multilayer thin film superstructures below and above the exchange bias blocking temperature. The ferromagnetic Co thin films are grown with the help of MBE at a base pressure of 10E-10 mbar whereas antiferromagnetic CoO thin films are grown from in-situ oxidized Co. The thicknesses of these films are monitored by reflection high energy electron diffraction (RHEED). A mean-field theory is outlined which provides an analytic and intuitive expression for the enhancement of the coercivity of the ferromagnet which experiences the exchange coupling with a neighboring antiferromagnet. An experimental approach is developed allowing to determine the interface susceptibility of an individual antiferromagnetic pinning layer by systematic change in the thickness of the antiferromagnet thin films in various sets of superlattice samples measured at different temperatures, respectively. The experiment enables us to separate out the intrinsic coercivity from the contribution induced by exchange coupling at the interface. It is the goal of our study to evidence or disprove if it is simply this susceptibility of the reversible interface magnetization creating the spin drag effect and by that the coercivity enhancement. Financial support by NSF through CAREER DMR-0547887, NRI and Nebraska MRSEC.
12:51PM J31.00007 Antiferromagnetic coupling in Fe/Si/Fe structures with Co “dusting” layers , RASHID GAREEV, MATTHIAS KIESLING, Uni Regensburg, MATTHIAS BUCHMEIER, Uni Muenster, GEORG WOLTERSDORF, CHRISTIAN BACK, Uni Regensburg, UNI REGENSBURG TEAM, UNI MUEENSTER COLLABORATION — Artificial antiferromagnetic (AF) tunneling Si-based structures are attracting a spatial interest due to extremely strong AF coupling, which exceeds 5μemu/m², low resistance-area product and resonant-type tunneling magnetoresistance (TMR) [1]. A promising way to regulate the spin polarization in TMR structures is to insert Co “dusting” layers at interfaces [2]. We present AF coupling in Fe/Co/Si/Co/Fe epitaxial structures with sub-monolayer—thick Co “dusting” layers at interfaces and different thicknesses of the Si spacer. We determined the strength of AF coupling from spin-wave frequencies and angular dependence of the resonance field of the ferromagnetic resonance, as well as MOKE hysteresis. We found the AF coupling near 0.1μemu/m² which decays with the spacer thickness and detectable for 2nm-thick Si spacers. The presented results can open an avenue for magnetotransport studies in AF-coupled structures using interface engineering. [1]. R.R. Gareev et al, JMMM 240, 235 (2002), R.R. Gareev et al, APL 88, 172105 (2006). [2]. Y. Wang, X.F. Han, and X.-G. Zhang, APL 93, 172501 (2008).

1:03PM J31.00008 Probing Magnetic Configurations in Buried Cobalt/Copper Multilayered Nanowires1, KAI LIU, University of California - Davis — Multilayered magnetic nanowires have been a model system for heterostructured junctions that exhibit a host of fascinating perpendicular spin transport phenomena, such as giant and tunneling magnetoresistance (MR), and spin-transfer torque effects. Due to the extremely small physical dimensions the magnetic components in these nanowires or junctions often exhibit complex magnetization reversal behaviors, which are difficult to probe by magnetic imaging since the entities are buried deep inside a matrix. Conventional hysteresis loop measurement alone cannot reliably distinguish the reversal mechanisms either. In this work we have captured magnetic and MR “fingerprints” of Co nanodiscs in Co/Cu multilayered nanowires as they undergo a single domain to vortex state transition, using a first-order reversal curve (FORC) method [1]. The nanowires have been electrochemically deposited into nanoporous polycarbonate membranes. In 50 nm diameter [Co(5nm)/Cu(8nm)]20 nanowires, a 10% MR effect is observed at 300 K. In 200 nm diameter nanowires, the magnetic configurations can be tuned by adjusting the Co nanodisc aspect ratio. Nanowires with thinnest Co exhibit single domain behavior. The nanowires show nucleation and annihilation of the vortices are manifested as butterfly-like features in the FORC distributions, similar to those observed in arrays of Fe nanodots [2]. They also show a superposition of giant and anisotropic magnetic interaction, which corresponds to the specific magnetic configurations of the Co nanodiscs.


1Work done in collaboration with Jared Wong, Peter Greene, Randy K. Dumas, Daniel Masiel, Nigel D. Browning, and June W. Lau, supported in part by NSF (ECCS-0725902 and PHY-0649297), CITRIS and the Alfred P. Sloan Foundation.

1:39PM J31.00009 Controlled formation of double-vortex configurations in a shape-engineered F/N/F trilayer stack studied by quantitative off-axis electron holography , LEI HUANG, MARVIN SCHOFIELD, YMEI ZHU, Department of Condensed Matter Physics and Material Science, Brookhaven National Lab — Vortex domain state, widely existing in submicron size patterned magnetic structures, can be very useful in high density magnetic magnetic data storage devices. In this report, we designed a shape engineered ferromagnetic-nonmagnetic-ferromagnetic (F/N/F) trilayer stack that would generate four different vortex-based remnant states by applying defined sequences of in-plane magnetic field. These four states are distinguished by different relative chirality orientations of two vortices stabilized in the ferromagnetic layers. Experimentally, we lithographically patterned 400nm sized prototype device, and studied in-situ the switching behavior by off-axis electron holography. Using the integrated approach including single element hysteresis loop, induction contour mapping and quantitative electron phase shift measurement, we revealed the underlying reversal mechanism as separate vortex formation and annihilation in two magnetic layers. We also confirmed the field-control feasibility of such structure by distinguishing unambiguously the presence of all four states after each field recipe was applied.

1:51PM J31.00010 Magnetic properties of ion-etched magnetic nanodot arrays , IOAN TUDOSA, KEITH CHAN, ERIK SHIPTON, ERIC FULLERTON, University of California San Diego — One pathway for increasing the density in magnetic recording media is to have bits stored as single patterned magnetic islands. While promising, this method has been hindered by the failure to reduce the island to island variation which decays with the spacer thickness and detectable for 2nm-thick Si spacers. The presented results can open an avenue for magnetotransport studies in AF-coupled structures using interface engineering. [1]. R.R. Gareev et al, JMMM 240, 235 (2002), R.R. Gareev et al, APL 88, 172105 (2006). [2]. Y. Wang, X.F. Han, and X.-G. Zhang, APL 93, 172501 (2008).

2:03PM J31.00011 Magnetic multilayers and Nanomagnetic Patterns , P. PANYAIJIRAWUT, M.S. RZ-CHOWSKI, University of Wisconsin-Madison — We have grown Ni/Co magnetic multilayers by sputtering, finding that the multilayers have in-plane uniaxial magnetic anisotropy. This is induced during growth by the sputtering geometry, and by the interaction between layers. We pattern the multilayers into sub-micron dots and networks using the nanosphere lithography technique, forming well-ordered two dimension arrays of magnetic nanoparticles. We use an oxygen plasma etch to adjust the size of the polystyrene spheres after spin coating. Using self-assembled close-packed monolayer of polystyrene spheres as deposition mask, the magnetic material is deposited through the interstitial areas to form networks. We also form isolated nanoparticles using the polystyrene spheres as aetch mask. We discuss the magnetic behavior of patterned multilayers.

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11:15AM J32.00001 Surface-state mediated indirect exchange interaction between magnetic nanodots on metallic substrates1, DI XIAO, LIFENG YIN, Oak Ridge National Laboratory, WENGUANG ZHU, U of Tennessee-Knoxville and Oak Ridge National Laboratory, G. MALCOLM STOCKS, JIAN SHEN, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory and U of Tennessee-Knoxville — We investigate theoretically the ferromagnetic ordering of magnetic nanodots grown on flat or vicinal metal substrates. We first show that, on a flat substrate, the surface state-mediated indirect exchange interaction between the nanodots can be significant enough to account for the high ferromagnetic transition temperature observed in recent experiments. We obtain the quantitative coupling strength and characteristic length scale of the magnetic interaction via detailed Monte Carlo simulations. We then study how the reduced dimensionality of the surface state on vicinal surfaces affects the collective magnetic behavior of the systems, and discuss the findings in connection with latest experimental observations.

1Supported by DMSE/BES of DOE and NSF.
11:27AM J32.00002 Artificial Nanomagnet With Lateral Confinement1. LIFENG YIN, ZHENG GAI, Oak Ridge National Laboratory, NOPPI WIDJAIA, Oak Ridge National Laboratory / The Univ. Tennessee, DI XIAO, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory / The Univ. Tennessee, WARD PLUMMER, The Univ. Tennessee / Louisiana State University, JIAN SHEN, Oak Ridge National Laboratory / The Univ. Tennessee — We introduce a novel way—curved Cu(111) substrate—to smoothly modify the surface states by introducing a miscut angle and study the impact of modifying vicinal surface states on the ferromagnetic behavior of Fe dots. With this curved substrate, the same growth parameter can be ensured in the whole miscut angle studied. When the Fe dot assemblies have an in-plane easy axis, two distinct regimes and a critical terrace width, separating these two regimes, can be identified. There are three contributing factors: the vicinal surface state, the competition between the Fe dots diameter and the terrace width, and the in-plane uniaxial magnetic anisotropy. The couplings between these three factors lead to the interesting behavior observed in the Fe/vicinal Cu(111) nanodot assemblies.

1Supported in part by the Division of Materials Science and Engineering, U. S. DOE.

11:39AM J32.00003 Multiple Quantum Transitions In Magnetic Nanoparticles. NATALIA NOGINOVA, NSU, Norfolk, VA, ADRIAN RADOCEA, Cornell University, Ithaca, NY, VADIM A. ATSARKIN, IRE, Moscow, Russia — Absorption at multiple resonance transitions of Fe/vicinal Cu(111) nanodot assemblies.

11:51AM J32.00004 SEMPA Measurements of Ferromagnetic Nanodisk Phase Diagrams. SEOK-HWAN CHUNG, CNST, NIST / Maryland NanoCenter. U. of Maryland, ROBERT MCMICHAEL, DANIEL PIERCE, JOHN UNGURIS, CNST, NIST — We use Scanning Electron Microscopy with Polarization Analysis (SEMPA) to image the magnetic domain structures of ferromagnetic nanodisks with different diameters and thicknesses, and thereby determine the phase diagram of the ground state in these technologically important magnetic structures. Depending on the nanodisk dimensions, one of three distinct ground state magnetic configurations is observed: a single domain in-plane, a single domain out-of-plane, or a vortex state. In contrast to previous work, the magnetic states of individual nanodisks are determined using simultaneous SEMPA measurements of both the in-plane and out-of-plane magnetization components. By systematically imaging Permalloy nanodisks with diameters that range from 35 nm to 190 nm and with thicknesses that range from 10 nm to 65 nm, we are able to locate phase boundaries and the triple point between these three phases. Near the phase boundaries and triple point we observe a mixture of the different phases. A model magnetic phase diagram generated by using the OOMMF micromagnetic simulator is found to agree well with the phase diagram determined by the SEMPA measurements. This work is supported by the NIST-CNST/UMD-NanoCenter Cooperative Agreement.

12:03PM J32.00005 Ordering, Texture and Magnetism in Ultrathin FePt Films. TOM GEORGE, XINGZHONG LI, RALPH SKOMSKI, DAVID J. SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska — Non-epitaxially grown L1₀ FePt ultrathin films have been fabricated and investigated. All films were magnetron sputtered onto SiO₂ substrates in the form [Fe/Pt]ₙ, with individual layer thicknesses from about 0.1 to 0.4 nm. The films' nominal total thickness ranged from 5 to 20 nm and was controlled by varying the number of bi-layer repetitions. The L1₀ phase and (001) texture were obtained by post-deposition annealing for 300 seconds at 600 °C. Transmission electron microscopy showed all as-deposited films as continuous; but after annealing, all films except the thickest ones showed agglomeration into a connected island-like morphology. L1₀ ordering and texture were confirmed by x-ray and electron diffraction, and the degree of order tended to decrease with increasing nominal film thickness. The (001) texture was greatest when the nominal film thickness was 12.5 nm, coinciding with an island thickness of the same value. SQUID magnetometry shows a relatively unusual trend of coercivity increasing with island thickness, with the highest value corresponding to the most ordered sample. The process of film agglomeration and the effects of bi-layer thickness and annealing temperature and time are also discussed. – This research is supported by NSF-MRSEC (RS), INSIC, DOE (DJS), and NCMN.

12:15PM J32.00006 Numerical Studies of Magnetization Reversal in Thin Anular Nanorings. GABRIEL CHAVES-O'FLYNN, ANDREW KENT, DANIEL STEIN, DANIEL BEDAU, New York University, NEW YORK UNIVERSITY TEAM — The rate of thermally activated magnetization reversal in thin ferromagnetic nanorings has been found analytically in a 1D model in which the demagnetization energy is approximated by a local surface term [1]. Numerical micromagnetic calculations confirm all aspects of the analytic model for narrow thin rings, such as peramally rings of 200 nm mean radius, 40 nm width and 2 nm thickness [2]. However, the model breaks down in for extremely wide rings, when the ring width approaches its mean diameter. Here we present numerical micromagnetic results for the transition states between the clockwise and counterclockwise state in this limit. We describe how the two transition configurations of narrow rings cease to be saddles of the energy functional. Also, a new low energy metastable state is found to exist for a narrow range of fields. We discuss the results of applying the String Method [3] to determine the transition states and energy barriers between the lowest magnetization configurations of rings. [1] K. Martens, D.L. Stein, and A.D. Kent, PRB 73, 054413 (2006) [2] G. D. Chaves-O’Flynn, D.L. Stein, and A.D. Kent, arXiv:0811.0440 (2008) [3] W. E, W. Ren, E. Vanden-Eijnden, J. Chem. Phys 126, 164103 (2007)

12:27PM J32.00007 Onset of magnetism in supported transition metal encapsulated silicon cages2. ROBERTO ROBLES, SHIV N. KHANNA, Dept. of Physics, Virginia Commonwealth University, Richmond, VA 23284 — In the past few years, silicon based clusters have attracted a lot of attention as building blocks of nanomaterials. Some of the most promising candidates are the transition metal encapsulated silicon cages, which have been shown to be specially stable, both experimentally and theoretically. However, for the use of these materials in fields like spintronics, it is not only necessary to be semiconductor based, but also that they present a finite magnetic moment. However, it has been shown that the magnetic moment of the transition metal atom encapsulated in silicon cages is quenched due to the hybridization with silicon. By performing density functional calculations in the generalized gradient approximation, we show that the magnetic moment of these clusters can be recovered by depositing them on a surface. Using CrSi₁₂ on Si(111) as an example, we have deposited the cluster in different orientations. The studies show that, for most of them, a finite magnetic moment is preserved in the system after a geometrical relaxation. The origin of this behavior is discussed in terms of hybridization, comparing to the unsupported situation.

2The authors are grateful to the Army Research Office for supporting this work through a MURI grant (Grant # W911NF-06-1-0280).
12:39PM J32.00008 Metamaterials with tunable refractive index fabricated from amorphous ferromagnetic microwires and optical Magnus effect\textsuperscript{1} , ANDREY IVANOV, ANATOLY VEDYAYEV, VLADIMIR GALKIN, ALEXANDER SHALYGIN, VALERY IVANOV, M.V. Lomonosov Moscow State University — For homogeneous NPVM (negative phase–velocity mediums) [V. G. Veselago, Soviet Physics - Uspekhi 10 (1968) 509; T. G. Mackay, A. Lakhtakia, Phys. Rev. E 69 (2004) 026602] anomalous effects such as negative refraction, light pressure, Doppler shift. Cherenkov-Vavilov radiation, Goos – Hänchen effects have been discovered in different frequency ranges. In this presentation the optical circular polarized effect is calculated for inhomogeneous mediums (optical Magnus effect) and it is shown that it is anomalous in NPVM with respect to “right-handed” materials. The proposed metamaterials fabricated from glass coated amorphous ferromagnetic Co-Fe-Cr-B-Si microwires are shown to exhibit a negative refractive index for electromagnetic waves over scale of GHz frequencies [A.V. Ivanov, A.N. Shalygin, A.V. Vedayev, V.A. Ivanov, JETP Letters 85 (2007) 565]. The magnetoelastic interaction between microwires has been taken into account. The phase and group velocities in proposed metamaterial have been calculated. The ratio of thereof depends monotonically on the size of the microwires. Optical properties of such metamaterials are tunable by an external magnetic field and mechanical stress.

\textsuperscript{1}This work is supported by RFBR (Russian Fund for Basic Research) Project 08-02-00830.

12:51PM J32.00009 Magnetism in 1D Cobalt-Cyclopentadienyl Sandwich Molecular Wire\textsuperscript{1} , HANNES ALLMAIER, Technical Univ. Graz, AT, C. MORARI, Univ. Catholique Louvain, DICE, Elect, BE, L. CHIONCEL, E. ARRIGONI, Technical Univ. Graz, AT, F. BEIUȘEANU, Univ. of Oradea, RO, A. LICHTENSTEIN, Univ. of Hamburg, DE, M. KATSNELSON, Univ. of Nijmegen, NL — A challenge for technological applications at the nanometer scale is to find magnetic materials with reduced dimensionality. Recent theoretical studies have predicted ferromagnetic and half-metallic behavior for the 1D-organic magnetic benzen vanadium wire. Here we discuss a variety of magnetic orderings such as antiferromagnetic and ferromagnetic half-metallicity in the cobaltocene Co2(C5H5)2 nanowire. We performed DFT-calculations to optimize its geometry and used the NMO downfolding technique to construct the real-space low energy Hamiltonian. To describe electronic correlations beyond the mean-field, we used the developed Variational Cluster Approach. Our preliminary results show that non-quasiparticle states appear in the half-metallic gap, which reduce considerably the spin polarization of such a wire. Ab-initio electron transport calculations are in progress to establish the role of cobaltocene nanowire as part of a future spin filter.

\textsuperscript{1}H.A., L.C and E.A. acknowledge support by FWF project P18505-N16.

1:03PM J32.00010 Comparative Density Functional study of Ti on CuN/Cu(100)\textsuperscript{1} , JESUS CRUZ, Georgetown University, PUSHPA RAGHANI, Stanford University, BARBARA JONES, IBM Almaden Research Lab — We have performed a Density Functional Theory (DFT) calculation using the Projector Augmented Wave (PAW) technique to study the electronic structure of adatoms of Ti placed on a single layer of copper nitride (CuN) surface grown on top of Cu(100). The insulating CuN surface mediates superexchange interactions between the magnetic adatoms, and also can strongly affect electronic properties. The PAW technique allows us to have elements of the precision of an all-electron (AE) calculation and the performance of an Ultrasonic Pseudopotential (USPPs) calculation. We compare results obtained of the magnetic moment, atomic positions, and charge densities of Ti adatoms with both USPPs and PAW methods, and discuss the similarities and differences between the methods. We also report studies of the effect of the Coulombic repulsion U in the PAW methodology, and compare some of these results to an all-electron calculation.

\textsuperscript{1}This work was supported by the Consejo Nacional de Ciencia y Tecnologia (CONACyT Mexico), the National Science Foundation (NSF) and the Stanford Center for Probing the Nanoscale (CPN).

1:15PM J32.00011 Characteristics of Co islets on Cu(111) from first principles calculations\textsuperscript{1} , DUY LE, TALAT RAMAN, University of Central Florida — Through first principles electronic calculations, based on the spin-polarized density functional theory using the generalized gradient approximation and the ultrasoft pseudopotential method in the plane wave representation, we have examined the structure and magnetic properties of Co monomer, dimer and several n-mers on Cu(111). We find that the monomer has slight preference for the fcc site as compared to the hcp (about 0.02eV) while there is no such preference in the case of the Co dimer. The dimer bond length is found to be about 2.15\textdegree. For the 6 atoms cluster, we find that it prefers to be antiferromagnetic and absolute magnetic moment of each Co atom is about 0.07-0.08\textmu B. The monomer is non-magnetic while a high magnetic moment of 1.94\textmu B per Co atom is found in the case of dimer. We discuss our results in the context of recent experimental and theoretical findings [1,2].


\textsuperscript{1}Work supported in part by DOE under Grant No DE-FG02-07ER46354.

1:27PM J32.00012 Growth and characterization of MnAs on HOPG , SHRIDHAR HEGDE, EVERETT FRASER, JAESUK KWON, HAO ZENG, HONG LUO, Department of Physics, University at Buffalo, SUNY — MnAs thin films grown on (110)-oriented metallic Fe nano-crystals at the interface and within the magnetite film under oxidizing conditions that result in pure magnetite growth on the FeO at 720\textdegree C thin films exhibit room temperature ferromagnetism and ferrimagnetic half-metallicity in the cobaltocene Co2(C5H5)2 nanowire. We performed DFT-calculations to optimize its geometry and used the non-quasiparticle states appear in the half-metallic gap, which reduce considerably the spin polarization of such a wire. Ab-initio electron transport calculations are in progress to establish the role of cobaltocene nanowire as part of a future spin filter.

\textsuperscript{1}Supported by DOE DE-FG-02-06ER46328

Superconductivity at $T_c$=38 K in Pristine and Sulfur Doped Amorphous Carbon

ZHIPING YIN, UC Davis, FRAÇOIS GYGI, Dept. of Applied Science, UC Davis, WARREN PICKETT, Department of Physics, UC Davis — The high temperature superconductivity (up to 25 K) observed in elemental Ca at high pressure extends across several phase boundaries, making understanding the crystal structures of Ca under high pressure of great importance. Above 100 GPa, both experiment and theory indicate three possible structures, having space groups $P4_{2}1_{2}1, Cmca$ and $Pnma$. The reported room temperature structure, primitive simple cubic in the 32-109 GPa range, is consistent with the calculations of multilayer crystallographic anisotropy. MOKE from these structures can have different sign depending on incidence angle; this is consistent with calculations of multilayer model. We found that the sign of MOKE can change also versus azimuthal angle, which was unexpected. Physics behind this phenomenon will be presented.

Competing s and d-wave superconducting order in V$_3$Si

SHANTANU MUKHERJEE, DANIEL AGTERBERG, University of Wisconsin-Milwaukee — Competing phases have generated a lot of interest in the study of cuprate and pnictide superconductors. Here we examine the competition between s and d-wave superconducting order in V$_3$Si. We provide microscopic arguments as to why both of these phases have a comparable transition temperature in this material. We further argue that many experimental probes provide evidence for this competition.

Theoretical study of FFLO phases and related phases in non-centrosymmetric superconductors

ZHICHAO ZHENG, DANIEL AGTERBERG — Superconducting order can break translational invariance, leading to a phase in which the Cooper pairs develop a coherent periodic spatially oscillating structure, such as in a FFLO phase. Some superconductors break inversion symmetry, leading to helical and multiple-q (FFLO-like) phases. We study these related phases with and without vortices. We show that for a FFLO phase, a crisscrossing lattice solution arises from the decay of conventional Abrikosov vortices into pairs of fractional vortices. We further show that the fractional vortex solution can also exist in the multiple-q phase of non-centrosymmetric superconductors.
12:15PM J33.00006 Non-centrosymmetric superconductor La$_3$Bi$_2$Pt$_3$, GABRIEL SEYFARTH, UCI & UdM, CIGDEM CAPAN, UCI, ANDREA BIANCHI, UdM, ZACHARY FISK, UCI, PIERRE RODIERE, CHRISTINE OPAGISTE, Institut Neel, Grenoble — Recently, we have discovered that the metallic La$_3$Bi$_2$Pt$_3$ (Y$_3$Au$_4$Sb$_5$ structure) becomes superconducting below a transition temperature $T_c$ of about 1.4K. Our interest in the superconducting phase of La$_3$Bi$_2$Pt$_3$ stems from the fact that it lacks a center of inversion, which may lead to unconventional superconductivity, including nodes in the superconducting gap function, even if the pair wave function exhibits the full spatial symmetry of the crystal. Compared to other non-centrosymmetric magnetic compounds in which superconductivity has recently been discovered, like CePt$_3$Si, UIr, CeRhSi$_3$ (under pressure), the nature of the superconducting state in La$_3$Bi$_2$Pt$_3$ is not complicated by strong electron correlations nor the coexistence of magnetism. This makes it a good model system to study superconductivity without inversion symmetry. In our presentation we will focus on the first basic characterization of our La$_3$Bi$_2$Pt$_3$ single crystals (X-ray, specific heat, resistivity, penetration depth, etc.).

12:27PM J33.00007 On d-Wave Superconductors with a Zeeman or Exchange Splitting of the Spin-Up and -Down Fermi Surfaces, CHIA-REN HU, Texas A&M University — For a given Zeeman (or exchange) energy $\hbar$, we used the Fermi-surface splitting, $\Delta_q$, as a variational parameter, and showed: (1) For an s-wave superconductor, the Sarma state is actually an unstable equilibrium state, which is known to exist for $0.5 < \hbar < 1$ only, and has energy higher than the un-polarized BCS state and the normal state. (2) For a d-wave superconductor, the Sarma-like state can actually exist down to $h=0$, and is a stable equilibrium state up to some $h_{\text{max}}$, if not considering other possible deformations of the order parameter (possibly symmetry breaking, such as going toward the FFLO state, which is known to exist at higher $h$ only), and its energy is lower than those of the un-polarized BCS state and the normal state. (3) The state can be further improved by introducing more variational parameters, which are still not symmetry-breaking. Thus we predict that for CeCoIn$_5$ and other d-wave superconductors the low-field superconducting state in a magnetic field parallel to the layers should already show some bulk spin-polarization, ad is NOT the usual un-polarized BCS state.

1The author acknowledges some summer support from Texas Center for Superconductivity at the University of Houston.

12:39PM J33.00008 Superconductivity from two dimensional interfaces: CuCl/Si, GaP/Si, ZnS/Si, S.H. RHIM, R. SANIZ, A. J. FREEMAN, Northwestern University — Two-dimensional (2D) interfaces of hetero-bonded semiconductor superlattices are studied using the highly precise FLAPW method. The 2D system, of metal-insulator-metal, is one of the candidate geometries to realize the excitonic mechanism of superconductivity, where $T_C$ can be greatly enhanced over phonon mediation. Epitaxially grown CuCl on Si (111) was reported to exhibit an anomalous diamagnetic susceptibility at 60-150 K. For all superlattices, 2D metallicity was found at the interfaces due to charge transfer from the polarity mismatch, as evidenced by their bands, Fermi surfaces, and charge densities. The $T_C$, calculated within the crude RMTA and the McMillan-Hopfield formula, is 0.5-4K in CuCl/Si. The $T_c$ vanishes for the other cases. To pursue the excitonic mechanism, we are determining the Kernel function $K(\omega)$, i.e. the average of the effective Coulomb interaction, with q dependent dynamic screening. First results for CuCl/Si show $K(\omega)$ to be attractive for a certain energy range.

1DOE (DE-F002-88ER45372/A022)
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12:51PM J33.00009 Standard Model for Superconductivity in Graphite Intercalation Compounds: Prediction of Optimum Standard $T_c$, YASUTAMI TAKADA, ISSP, University of Tokyo — Based on the model that was successfully applied to the explanation of superconductivity with the transition temperature $T_c$ of about 0.1K or less in the alkali-intercalated graphite compounds such as K$_x$C, Rb$_x$C, and Cs$_x$C in 1982 [Y. Takada, J. Phys. Soc. Jpn. 51, 63 (1982) ], we have calculated $T_c$ for the alkaline-earth-intercalated graphite compounds including Ca$_y$C, Ba$_y$C, and Sr$_y$C, with $T_c$ of about 10K or less to find that the same model reproduces the observed $T_c$ in those compounds as well, indicating that it is a standard model for superconductivity in the graphite intercalation compounds with $T_c$ ranging over three orders of magnitude. The difference in $T_c$ by two orders between K$_x$C and Cs$_x$C can be accounted for by (i) doubling the valency of the metal ions, which enhances $T_c$ by one order, and (ii) tripling the effective mass of the superconducting three-dimensional electrons in the interlayer band, which also enhances $T_c$ by one order. Enhancement of $T_c$ well beyond 10 K is also predicted in this model, if intercalant metals are judiciously chosen so that both $Z$ and $m^*$ are increased further.

10:03PM J33.00010 Crystal structure and physical properties of new layered oxysulfides (Cu$_2$S$_2$)(Sr$_5$Sc$_2$O$_6$)$_3$, (Cu$_2$S$_2$)(Ba$_3$Sc$_2$O$_6$) and (Cu$_2$S$_2$)(Ba$_3$In$_2$O$_5$), HIARUKO OGINO, KOICHI USHIYAMA, YUKARI KATSURA, SHIGEORI HORII, JUN-ICHI SHIMOYAMA, KOJII KISHIO — Recently high-$T_c$ superconductors were discovered in layered oxynitride systems with stacking of fluorescent oxide layers and anti-fluorite-like nitride layers. Materials having similar stacking structure with perovskite-based oxide layers. Structural features and physical properties of these new materials will be presented.

1:15PM J33.00011 High-$T_c$ superconductivity in nanostructured Na$_x$WO$_{3-y}$; Sol-gel route, ALI ALIEV, NanoTech Institute, University of Taxis at Dallas, Richardson, TX 75083 — Tungsten trioxide, WO$_3$, infiltrated into various nanoporous matrix structures such as carbon inverse opal, carbon nanotubes paper, or platinum sponge and then intercalated with alkaline ions (Li$, Na$) exhibits a pronounced diamagnetic onset in ZFC magnetization in a wide range of temperatures, 125-123 K. Resistivity measurements show non zero jump and intensive fluctuations of electrical resistance below observed transition points. The observed magnetic and electrical anomalies in nanostructured tungsten bronzes (Li$^x$WO$_{3-y}$, Na$^x$WO$_{3-y}$) suggest the possibility of localized non-percolated superconductivity. The direct evidence of polaron formation from temperature dependence of EPR and photoemission spectra and formation of bipolarons in weakly reduced to WO$_{3-y}$, with y typically in the order of 2.95 suggest bipolarons mechanism of a Bose-Einstein condensation of trapped electron pairs in doped WO$_{3-y}$. On the other hand the strong lattice instabilities in 2D systems like layered cuprates and tungsten bronzes place the upper limit on $T_c$. Than, the percolative self-organized mechanism on the metal/insulator interface like Na$^x$WO$_3$ and NaWO$_3$/nanostructured matrix can facilitate the high $T_c$ obtained in sodium bronzes infiltrated into inverted carbon opal or carbon nanotube matrices.
deposited on the surface at room temperature, and the resultant Na\(^+\)WO\(_3\) state drastically increased. The same behavior was observed for pure WO\(_3\). Charge transfer to the WO\(_3\) superconductivity in surface-doped WO\(_3\).

HAMMOND, THEODORE GEBALLE, MALCOLM BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University — We report the search for superconductivity in surface-doped WO\(_3\) films. Possible evidence for high temperature superconductivity in this system has been reported in the literature. In our work, WO\(_3\) films were grown by MBE and characterized by in-situ XPS, UPS, and ex-situ XRD and resistivity measurements. For some films, Na was deposited on the surface at room temperature, and the resultant Na\(^+\)WO\(_3\) films annealed in vacuum (\(\sim 10^{-8}\) Torr) for 1h at various temperatures (300 – 800°C). With increasing thickness of Na, the intensity of the Na\(^+\) peak in XPS spectra and area of the W5d state in UPS spectra increased, suggesting some charge transfer to the WO\(_3\) film. After annealing below 500°C, XPS and UPS spectra did not change, while after annealing above 500°C, the area of the W5d state drastically increased. The same behavior was observed for pure WO\(_3\) films, however, suggesting that oxygen vacancies are created during the annealing. The films started to decompose above 700°C. The resistivity of our films decreased with increasing annealing temperature. However, so far we have not observed any sign of superconductivity down to 2 K in any of our films. This work is supported by Air Force Office of Scientific Research.

Tuesday, March 17, 2009 11:15AM - 1:51PM –
Session J34 DCMP: Focus Session: Iron Pnictides and Other Novel Superconductors VII: Pressure Effects and Thermal Expansion 404

11:15AM J34.00001 Effects of pressure on CaFe\(_2\)As\(_2\) and related materials\(^1\), PAUL CANFIELD, Ames Lab / Iowa State University — The discovery of CaFe\(_2\)As\(_2\)\(^2\) and its extreme pressure dependence \(^2\) (even for pressures below 1 GPa) has lead to it being used as a model system for understanding the effects of pressure on the (AE)Fe\(_2\)As\(_2\) (AE = Ba, Sr, Ca) compounds.\(^3\) We have found that the combination of extreme pressure sensitivity with a first order structural phase transition that involves significant changes in the unit cell dimensions makes CaFe\(_2\)As\(_2\) very sensitive to the pressure medium used. In liquid medium, self clamping cells the higher temperature transitions, while generally detectable and highly reproducible\(^4\) are smeared and broadened, especially near the first order phase transition between the low temperature orthorhombic and collapsed tetragonal phases. In He-pressure cells these transitions remain extremely sharp.\(^5\) Superconductivity is detected between \(\sim 0.3\) and \(\sim 0.7\) GPa in the liquid medium cells and is essentially absent in the He-pressure cell.\(^5\) This superconducting region can be associated with a coexistence of low temperature phases brought on by non-hydrostatic components associated with the medium’s inability to respond to the high-temperature structural phase transitions.\(^5\) The origin of the superconductivity in this mixed region remains a topic of keen experimental and theoretical interest.


\(^{1}\)Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

11:51AM J34.00002 Discovery of a pressure-induced “collapsed” phase in CaFe\(_2\)As\(_2\), A. KREYSSIG,\(^1,2\),\(^2\)
\(^{1}\)Ames Laboratory; \(^^{2}\)Dep. of Materials Science and Engineering, University of Maryland, College Park, Y. LEE, G.D. SAMOLYUK, Z. JIANG, B. NIST Center for Neutron Research, Gaithersburg; \(^{4}\)Dep. of Physics, San Diego State University, San Diego, N. NI, S. NANDI, J.B. LEÃO, S.J. POULTON, D.N. ARGYRIOU, \(^{6}\)Helmholtz-Zentrum Berlin fuer Materialien und Energie, Germany, B.N. HARMON, R.J. MCQUEENI, A.I. GOLDMAN, — Recent investigations of the superconducting iron-arsenide families have highlighted the role of pressure, be it chemical or mechanical, in forming superconductivity. \(^{5}\) We report that CaFe\(_2\)As\(_2\) undergoes a pressure-induced transition to a non-magnetic, volume “collapsed” tetragonal phase, which becomes superconducting at lower temperature. Spin-polarized total-energy calculations on the collapsed structure reveal that the magnetic Fe moment itself collapses, consistent with the absence of magnetic order in neutron diffraction. – The support by U.S. DOE (DE-AC02-07CH11358) and NSF (DMR-0306165 and DMR-0805335) is acknowledged.

12:03PM J34.00003 Pressure-induced superconducting state of CaFe\(_2\)As\(_2\) from an antiferromagnetic spin-density wave state, HANOH LEE, EUNSUNG PARK, TUSON PARK, F. RONNING, E.D. BAUER, J.D. THOMPSON, Los Alamos National Laboratory — The spin-density-wave (SDW) antiferromagnet CaFe\(_2\)As\(_2\) has been reported as superconducting under pressure. By measuring electrical resistivity and magnetic susceptibility under pressure in silicon fluid as a pressure medium, we show that bulk superconductivity is present in a narrow pressure range where orthogonal and collapsed tetragonal state coexist. At higher pressures, where the collapsed tetragonal structure is proposed, distinctive electrical resistivity and magnetic susceptibility under pressure are observed, consistent with the absence of magnetic order in neutron diffraction. – The support by U.S. DOE (DE-AC02-07CH11358) and NSF (DMR-0306165 and DMR-0805335) is acknowledged.

12:15PM J34.00004 Structural changes in pressure induced superconducting BaFe\(_2\)As\(_2\), SIMON KIMBER, Helmholtz-Zentrum Berlin fur Materialien und Energie (HZB), ANDREAS KREYSSIG, Ames Laboratory, US DOE, Iowa State University, Ames, IA 5001, USA, FABIANO YOKAIKIYAMA, DIMITRI ARGYRIOU, Helmholtz-Zentrum Berlin fur Materialien und Energie (HZB), JIAQIANG YAN, Ames Laboratory, US DOE, Iowa State University, Ames, IA 5001, USA, THOMAS HANSEN, Institute Max von Laue-Paul Langevin, 6 rue Jules Horowitz, TAPAN CHATTERJI, JCNS, Forschungszentrum Julich Outstation at Institut Laue-Langevin, ROBERT MCQUEENI, PAUL CANFIELD, ALAN GOLDMAN, Ames Laboratory, US DOE, Iowa State University, Ames, IA 5001, USA — We have determined the crystal structure of BaFe\(_2\)As\(_2\) as a function of pressure (0 – 150 kbar) and pressure (0 – 6 GPa) using neutron powder diffraction. The structural features important to superconductivity, namely suppression of the T-O phase transition and reduction in the As-Fe-As bond angle and Fe-Fe distance, show exactly the same behaviour under pressure up to the optimal \(T_c\) value, as found in chemical doped samples. This result suggests that chemical doping and pressure have similar effects on the electronic degrees of freedom in this family of iron pnictide superconductors.
12:27PM J34.00005 Diffraction Studies of the P-T Phase Diagram with Single-Crystal Ca122
A.I. GOLMAN, A. KREYSSIG, Ames Laboratory/Department of Physics and Astronomy, K. PROKES, Helmholtz-Zentrum Berlin für Materialien und Energie, D.K. PRATT, Ames Laboratory/Department of Physics and Astronomy, D.N. ARGYRIOU, Helmholtz-Zentrum Berlin für Materialien und Energie, J.W. LYNN, NCNR, Gaithersburg, MD 20899, S. NANDI, Ames Laboratory/Department of Physics and Astronomy, S.A.J. KIMBER, Helmholtz-Zentrum Berlin für Materialien und Energie, Y. CHEN, NCNR, Gaithersburg, MD 20899, Y.B. LEE, G. SAMOLYUK, Ames Laboratory/Department of Physics and Astronomy, J.B. LEAO, S.J. POURTON, NCNR, Gaithersburg, MD 20899, S.L. BUDKO, N. NI, P.C. CANFIELD, B.N. HARMON, R.J. MCQUEENEY, Ames Laboratory/Department of Physics and Astronomy — Single crystal neutron and high-energy x-ray diffraction have identified the phase lines corresponding to transitions between the ambient-pressure tetragonal (T), the antiferromagnetic orthorhombic (O) and the nonmagnetic collapsed tetragonal (cT) phases of CaFe2As2. We find no evidence of additional structures for pressures up to 2.5 GPa (at 300 K). Both the T-c and O-c transitions exhibit significant hysteresis effects and we demonstrate that coexistence of the O and cT phases can occur if a non-hydrostatic component of pressure is present.

12:39PM J34.00006 Pressure-induced shift of $T_c$ in $K_xSr_{1-x}Fe_2As_2$ ($x = 0.2, 0.4, 0.7$): Analogy to the high-Tc cuprate superconductors, MELISSA GOOCH, Texas Center for Superconductivity at the University of Houston and Department of Physics, BING LV, Texas Center for Superconductivity at the University of Houston and Department of Chemistry, BERND LORENZ, Texas Center for Superconductivity at the University of Houston and Department of Physics, ARNOLD GULOY, Texas Center for Superconductivity at the University of Houston and Department of Chemistry, CHING-WU CHU, Texas Center for Superconductivity at the University of Houston; Lawrence Berkeley National Laboratory; Hong Kong University of Science and Technology — Through a systematic study of $K_xSr_{1-x}Fe_2As_2$ ($x = 0.2, 0.4, 0.7$), by pressure shifts of the $T_c$, similarities between the FeAs and high Tc superconductors can be observed. These similarities develop directly from the layered structure seen in both superconductors, which consists of an active superconducting layer and a charge reservoir block. The pressure coefficient of $T_c$ depends on the doping level: $dT_c/dp > 0$ (underdoped, $x = 0.2$), $dT_c/dp = 0$ (optimally doped, $x = 0.4$), and $dT_c/dp < 0$ (overdoped, $x = 0.7$). This is understood in terms of a pressure-induced charge transfer between the active and charge reservoir layers. In addition to the measured pressure shift in the $T_c$, the suppression of the spin density wave can clearly be demonstrated for the $x = 0.2$ case.

12:51PM J34.00007 Pressure Effect on the Structural and Magnetic Transition in CaFe$_2$As$_2$, SHILIANG LI, University of Tennesse, YING CHEN, NIST Center for Neutron Research, University of Maryland, JEFFREY LYNN, NIST Center for Neutron Research, XIANHUI CHEN, University of Science and Technology, PENGCHENG DAI, University of Tennessee, RK. BEWLEY, T. GUIDI, ISIS, Rutherford University Lab. — Application of ~2.5 kbar pressure induces superconductivity in CaFe$_2$As$_2$ with a $T_c$ of ~12K that remains constant up to ~7kbar, where superconductivity is again suppressed. This modest pressure enables the use of neutron scattering to study in detail changes of the spin and lattice correlations between normal and superconducting state as a function of pressure. The elastic part of the scattering measured on the MERLIN spectrometer utilizing a He gas pressure cells shows that at 4kbar pressure and 2k only ~50% of the sample has transformed to the collapsed tetragonal phase. The inelastic spectra show a suppression of spectral weight at low energies and small momentum transfer on going from ambient pressure to the superconducting state at 4kbar and 2k. The spectral weight is transferred to higher energies and wavevectors, leading to a V-shaped excitation branch in the collapsed tetragonal phase. Work supported by US DOE BES-DEMS-AC02-06CH11357.

1:03PM J34.00008 Pressure dependence of the inelastic neutron scattering response of CaFe$_2$As$_2$, S. ROSENKRANZ, R. OSBORN, E. GOREMYCHKIN, I.S. Todorov, D.Y. CHUNG, H. CLAUS, J.A. SCHLUETER, Argonne Nat. Lab., C.D. MALLIAKAS, M.G. KANATZIDIS, Northwestern Univ., A.D. CHRISTIANSON, Oak Ridge Nat. Lab., R.I. BEWLEY, T. GUIDI, ISIS, Rutherford University Lab. — Application of ~2.5 kbar pressure induces superconductivity in CaFe$_2$As$_2$ with a $T_c$ of ~12K that remains constant up to ~7kbar, where superconductivity is again suppressed. This modest pressure enables the use of neutron scattering to study in detail changes of the spin and lattice correlations between normal and superconducting state as a function of pressure. The elastic part of the scattering measured on the MERLIN spectrometer utilizing a He gas pressure cells shows that at 4kbar pressure and 2k only ~50% of the sample has transformed to the collapsed tetragonal phase. The inelastic spectra show a suppression of spectral weight at low energies and small momentum transfer on going from ambient pressure to the superconducting state at 4kbar and 2k. The spectral weight is transferred to higher energies and wavevectors, leading to a V-shaped excitation branch in the collapsed tetragonal phase. Work supported by US DOE BES-DEMS-AC02-06CH11357.


1:27PM J34.00010 High-Resolution Thermal Expansion Measurements of CaFe$_2$As$_2$, ARIANA DE CAMPOS, M.S. DA LUZ, J.J. NEUMEIER, Montana State University, E.D. BAUER, F. RONNING, J.D. THOMPSON, HANOH LEE, TUSON PARK, Los Alamos National Laboratory, EUNSYUNG PARK, Sungkyunkwan University — The discovery of superconductivity in doped LaFeAsO initiated a surge of interest in layered FeAs systems. The recent discoveries in CaFe$_2$As$_2$ [1,2] of: (i) suppression of the first-order structural phase transition under modest hydrostatic pressure, (ii) superconductivity under pressure and (iii) at higher pressures the suppression of superconductivity with stabilization of a potentially different high temperature phase, establish pressure as a valuable parameter for tuning the behavior of these fascinating compounds. In this work, thermal expansion measurements of a high-quality single crystal of CaFe$_2$As$_2$ are reported. A sharp transition was observed between the high temperature tetragonal and low temperature orthorhombic structures at $T_s = \approx 180$ K. [1] M.S. Torikachvili, et al. PRL 101, 057006(2008). [2] Park T., et al., J. Phys.Cond.Matter, 20, 32204 (2008). This material is based upon work supported by the Brazilian Agency CNPq (Grant No. 201439/2007-7), the NSF (Grant No. DMR-0504769) and U.S. DOE Office of Basic Energy Sciences (Grant No. DE-FG-06ER46209). Work at LANL was performed under the auspices of the U.S. DOE Office of Basic Energy Sciences and supported by the LDRD program.

1:39PM J34.00011 Magnetic Ordering and Negative Thermal Expansion in PrFeAsO, D.N. ARGYRIOU, S.A.J. KIMBER, F. YOKAICHYA, K. HABICH, S. GERISCHER, Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Glienicker Strasse 100, D-14109, Germany, R. KLINGELER, C. HESS, G. BEHR, A. KONDRAT, B. BUCHNER, Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, Germany, T. HANSEN, T. CHATTERJI, Institute Max von Laue-Paul Langevin, 6 rue Jules Horowitz, BP 156, F-38042, Grenoble Cedex 9, France — We report the structure and magnetism of PrFeAsO; one of the parent phases of the newly discovered Fe-As superconductors, as measured by neutron powder diffraction. In common with other REFeAsO materials, a tetragonal-orthorhombic phase transition is found on cooling below 136 K and striped Fe magnetism with $k = (1,0,1)$ is detected below $\sim 85$ K. Our magnetic order parameter measurements show that the ordered Fe moment along the $a$ axis reaches a maximum at $\sim 40$ K, below which an anomalous expansion of the $c$ axis sets in, which results in a negative thermal volume expansion of 0.015% at 2 K. We propose that this effect, which is suppressed in superconducting samples, is driven by a delicate interplay between Fe and Pr ordered moments.
Tuesday, March 17, 2009 11:15AM - 2:03PM
Session J35 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors VIII: Magnetism (Experiment) 405

11:15AM J35.00001 Nuclear and Magnetic structures of CeFeAs$_1$-$x$P$_x$O. CLARINA DELA CRUZ, PENGCHENG DAI, Univ. of Tennessee and NSSD-ORNL, HERBERT MOOK, NSSD-ORNL, Q. HUANG, M. GREEN, J. LYNN, NIST NCNR, N.L. WANG, G.F. CHEN, J.L. LOU, IPCAS — A new class of superconductors (RO$_1$-$x$F$_x$FeAs) has been discovered very recently which has resulted to a flurry of activities in the scientific community. Our initial work on the La based parent compound successfully revealed, for the first time, the AFM order which is preceded by a structural distortion from tetragonal to orthorhombic nuclear structures. A model for the magnetic structure was also proposed. Both magnetic order and structural distortion are suppressed in lieu of the superconducting phase. Our systematic study of the doping dependence of both the nuclear and magnetic structure of CeO$_1$-$x$P$_x$FeAs as well as in the La system has established the nature of the competition between the static AFM order of the Fe spins and the superconductivity. This work looks at the effects of the tuning of the structural parameters in the compounds without doping carriers into the system. This is motivated by the belief that structurally driven electronic effects are very important in these highly correlated systems. We study the parent compound CeFeAsO and change the particulars about the structural distortion by substituting P on the As site until it’s approach to CeFePO which is a nonmagnetic heavy Fermion. We present interesting details of the phase diagram of CeFeAs$_1$-$x$P$_x$O with respect to the As/P concentration.

11:27AM J35.00002 Lattice and magnetic instabilities in CaFe$_2$As$_2$. SHIBABRATA NANDI, ALAN GOLDMAN, Ames Laboratory, US DOE and Iowa State University, DIMITRI ARGYROIU, Helmholtz-Zentrum Berlin fur Materialien und Energie, BACHIR OULADDIF, Institute Laue-Langevin, TAPAN CHATTERJI, Forschungszentrum Julich Outstation at Institute Laue-Langevin, ANDREAS KREYSSIG, NI NI, SERGEY BUD’KO, PAUL CANFIELD, ROBERT MCQUEENEY, Ames Laboratory, US DOE and Iowa State University. Neutron diffraction measurements of a high quality single crystal of CaFe$_2$As$_2$ are reported. A sharp peak in the high temperature tetragonal and low temperature orthorhombic structures at $T_S=172.5$ K (on cooling) and 173.5 K (on warming). Concomitant with the structural transition we observe a rapid, but apparently continuous, ordering of the Fe moments, in a commensurate antiferromagnetic structure, with a saturated moment of 0.80(5) $\mu_B$/Fe directed along the orthorhombic a-axis. The hysteresis of the structural transition is 1 K between cooling and warming and is consistent with previous thermodynamic, transport and single crystal x-ray studies. The temperature onset of magnetic ordering shifts rigidly with the structural transition providing clearest evidence to date of the coupling between the structural and magnetic transitions in this material and the broader class of arsenides.

11:39AM J35.00003 High Energy Spin Waves in CaFe2As2 Single Crystals, SOULEYMANE DIALLO, VLADIMIR ANTROPOV, Ames Laboratory, COLLIN BROHOLM, Johns Hopkins University, TOBY PERRING, ISIS Neutron Facility, SERGEY BUD’KO, Ames Laboratory, NI NI, Iowa State University, PAUL CANFIELD, Ames Laboratory, ANDREAS KREYSSIG, kreyssig@ameslab.gov, ALAN GOLDMAN, ROBERT MCQUEENEY, Ames Laboratory — We present neutron scattering measurements of the magnetic excitations in single crystals of antiferromagnetic ordered CaFeAs$_2$ (TN = 172 K), the parent compound of the newly discovered iron-arsenide based superconductors. The data reveals steeply dispersive and well-defined spin waves up to an energy of approximately 120 meV. The data below 120 meV can be fit to a Heisenberg model consisting of nearest-neighbor interactions (J$_1$a, J$_1$b and J$_1$c) and next-nearest neighbor interaction (J$_2$), yielding constraining values on the magnetic exchange coupling constants. Above 120 meV, the excitations appear weaker or strongly damped. Ab-initio calculations of the dynamic magnetic susceptibility show that the high energy behavior arises from the damping of itinerant spin waves by particle-hole excitations.

11:51AM J35.00004 Neutron Scattering Study of the Fe Oxypnictide Superconductors NdFeAsO$_{1-x}$F$_x$ and LaFeAsO$_{0.87}$F$_{0.13}$. YIMING QIU, NIST Center for Neutron Research and Univ. of Maryland, WEI BAO, QINGZHENG HUANG, TANER YILDIRIM, JASON SIMMONS, MARK GREEN, YING CHEN, JEFF LYNN, MAIKO KOFU, SEUNGHUN LEE, T. WU, G. WU, XIANHUI CHEN — We report the neutron scattering studies of NdFeAsO$_{1-x}$F$_x$ ($x=0, 0.2$)[1] and LaFeAsO$_{0.87}$F$_{0.13}$[2]. In NdFeAsO, there is a tetragonal to orthorhombic structural transition at $T_S=150$ K, where an anomaly in resistivity also occurs. A long range magnetic order with the wave-vector (1/2, 1/2, 0) forms below $T_N=1.96$ K. This long range order is dominated by the rare earth Nd ions, however, both the Nd and smaller Fe moments contribute to the antiferromagnetic structure. Neither the magnetic ordering nor the structural distortion occurs in the superconducting samples NdFeAsO$_{0.80}$F$_{0.20}$ and LaFeAsO$_{0.87}$F$_{0.13}$ at temperatures down to 1.6 K. In LaFeAsO$_{0.87}$F$_{0.13}$, no magnetic-resonance peak was observed in the superconducting state at 1.6 K. Two phonon peaks at 12 and 17 meV were observed, consistent with theoretical calculation. Reference: [1] Y. Qiu et al., arXiv:0806.2195 accepted by PRL(2008) [2] Y. Qiu et al., Phys. Rev. B 78, 052508(2008)

1Supported by NSF, US DOE, NSF of China, Ministry of Science and Technology of China, National Basic Research Program of China.

12:03PM J35.00005 The crystalline electric field as a probe for long range antiferromagnetic order and superconductivity in CeFe$_2$As$_2$. SONGXUE CHI, University of Tennessee, Knoxville, DEVASHIBHAI ADROJA, ISIS Facility, Rutherford Appleton Laboratory, TITIANA GUIDI, ROBERT BEWLEY, ISIS Facility, Rutherford Appleton Laboratory, SHI LIANG LI, JUN ZHAO, University of Tennessee, JEFFREY LYNN, CRAIG BROWN, YIMING QIU, NIST Center for Neutron Research, GEN FU CHEN, JIAN LIN LUO, NAN LIN WANG, Institute of Physics, Chinese Academy of Sciences, PENGCHENG DAI, University of Tennessee, Knoxvill — We use inelastic neutron scattering to study the crystalline electric field (CEF) excitations of Ce$^{3+}$ in CeFeAs$_{1-x}$F$_x$($x=0,0.10$). For nonsuperconducting CeFeAsO, the Ce CEF levels have two magnetic doublets in the paramagnetic state, but these doublets split into six singlets when Fe ions order antiferromagnetically. For superconducting CeFeAsO$_{0.84}$F$_{0.16}$ ($T_c=41$ K), where the static AF order is suppressed, the Ce CEF levels have three magnetic doublets at all temperatures. Careful measurements of the intrinsic linewidth and the peak position of the 18.7 meV mode reveals clear anomaly at $T_c$. These results suggest that CEF excitations in the rare-earth oxypnictides can be used as a probe of spin dynamics in the nearby FeAs planes.

1This work is supported by the US DOE BES through DOE DE-FG02-05ER46202.

12:15PM J35.00006 Inelastic neutron scattering studies on spin excitations of Fe Pnictides. JUN ZHAO, Department of Physics and Astronomy, The University of Tennessee, DAO-XIN YAO, Department of Physics, Purdue University, SHI LIANG LI, Department of Physics and Astronomy, The University of Tennessee, TAO HONG, Neutron Scattering Science Division, Oak Ridge National Laboratory, YING CHEN, SUNG CHANG, WILLIAM RÄTLIFF, JEFF LYNN, NIST Center for Neutron Research, National Institute of Standards and Technology, HERBERT MOOK, Neutron Scattering Science Division, Oak Ridge National Laboratory, GENFU CHEN, JIANLIN LUO, NANNING WANG, Institute of Physics, Chinese Academy of Sciences, JINGCHUN HU, Department of Physics, P. CARL UNÖVER, JUN ZHAO, ZHANGHONG LIU, Department of Physics, P. CARL UNÖVER, JUN ZHAO, ZHANGHONG LIU, Department of Physics, Oak Ridge National Laboratory, The University of Tennessee & Neutron Scattering Science Division, Oak Ridge National Laboratory — We used inelastic neutron scattering to study the evolution of spin excitations in the FeAs superconductors and their parent compounds. We show here not only the antiferromagnetic order is suppressed by the doping; the spin excitations also change dramatically with doping. We observed sharp spin-wave excitations in the antiferromagnetically ordered parent compound. Based on the observed dispersion relation, we estimate the effective magnetic exchange coupling using a Heisenberg model. We also studied the spin excitation spectrum in the superconducting sample and its relationship to the superconductivity.
12:27PM J35.00007 Resonant spin excitation in Ba$_{1-x}$K$_x$Fe$_2$As$_2$†, R. OSBORN, S. ROSENKRANZ, E.A. GORE-MYCHKIN, D.Y. CHUNG, I.S. TODOROV, H. CLAUS, Argonne National Laboratory, A.D. CHRISTIANSON, M.D. LUMSDEN, Oak Ridge National Laboratory, C.D. MALLIAKAS, M.G. KANATZIDIS, Northwestern University, R.I. BEWLEY, T. GUIDI, ISIS Pulsed Neutron and Muon Facility — In the iron arsenides, superconductivity occurs when the antiferromagnetism of a parent compound has been suppressed by chemical doping. We have investigated the evolution of the magnetic response with potassium doping in Ba$_{1-x}$K$_x$Fe$_2$As$_2$. In the parent compound (x = 0), there is evidence of a column of inelastic scattering at the AF wavevector, Q$_{AF}$ = 1.2Å$^{-1}$, consistent with a steep dispersion of gapped spin waves. A similar inelastic column is seen in the normal phase in the z = 0.4 compound, but it persists to lower energy transfer. However, at the superconducting transition of 38K there is a transfer of spectral weight into an excitation localized at Q$_{AF}$ = 1.2Å$^{-1}$ and ω = 14meV [A. D. Christianson et al, Nature, in press]. Such resonant spin excitations, which are a universal feature of the copper oxide superconductors and seen in several heavy fermion superconductors, provide evidence that the energy gap has unconventional symmetry, with opposite sign on portions of the Fermi surface connected by the resonance wavevector.

†Work supported by US DOE BES-DBM DE-AC02-06CH11357.

12:39PM J35.00008 Antiferromagnetic spin correlations in the tetragonal phase of CaFe$_2$As$_2$‡, R.J. MCQUEEN, S.O. DIALLO, J.L. ZARESTKY, Ames Laboratory, US DOE and Iowa State University, C. BROHOLM, Johns Hopkins University, T.G. FERRING, Rutherford Appleton Laboratory, S.L. BUD’KO, N. NI, A. KREYSSIG, P.C. CANFIELD, A.I. GOLDMAN, Ames Laboratory, US DOE and Iowa State University — We present neutron scattering measurements of magnetic excitations in the tetragonal phase of CaFe$_2$As$_2$. Below T$_S$ = 173 K, CaFe$_2$As$_2$ undergoes a first-order transition to an orthorhombic structure with columnar antiferromagnetic ordering with a wavevector Q$_{AFM}$ = (101). This phase is characterized by strong magnetic interactions giving rise to steep spin waves. In the tetragonal phase above T$_S$, broad quasi-elastic excitations are observed near Q$_{AFM}$ that display a weak dependence on L, indicating two-dimensional antiferromagnetic correlations. These correlations are observed to persist up excitation energies of ~50 meV and temperatures of at least 300 K. Our results indicate that strong magnetic interactions exist above T$_S$, and ordering is likely suppressed by magnetic frustration.

‡Work supported by US DOE BES-DBM DE-AC02-06CH11357; at USTC by National Science Foundation of China & Ministry of Science and Technology of China & National Basic Research Program of china; at LANL by U.S. DOE/OS.

12:51PM J35.00009 Magnetic order the iron spins in NdOFeAs, YING CHEN, NCNR and Univ. of Maryland, J.W. LYNN, NCNR, J. LI, NCNR and Univ. of Maryland, G. LI, G.F. CHEN, J.L. LUO, N.L. WANG, Chinese Academy of Sciences, PENGCHENG DAI, C. DELA CRUZ, Univ. of Tennessee & ORNL, H.A. MOOK, ORNL — Polarized and unpolarized powder neutron-diffraction measurements have been carried out to investigate the magnetic order in one of the highest Tc system, NdFeAsO. Antiferromagnetic order is observed below 141 K [1], which is in close proximity to the structural distortion observed in this material [2]. The magnetic structure consists of chains of parallel spins that are arranged antiparallel between chains, which is the same in-plane spin arrangement as observed in all the other iron oxypnictide materials. Nearest-neighbor spins along the c axis are antiparallel like LaFeAsO [3]. The ordered moment is 0.25 (7) μB, which is the smallest ordered moment found so far in these systems.


1:03PM J35.00010 Coexistence of the spin-density-wave and superconductivity in the Ba$_{1-x}$K$_x$Fe$_2$As$_2$ system, YANG REN, APS, Argonne National Laboratory, H. CHEN, University of Science and Technology of China, Y. QIU, NIST Center for Neutron Research & Univ. of Maryland, WEI BAO, Los Alamos National Laboratory, R.H. LIU, G. WU, T. WU, Y.L. XIE, X.F. WANG, University of Science and Technology of China, Q. HUANG, NIST for Neutron Research, NIST, X.H. CHEN, University of Science and Technology of China — The relation between the spin-density-wave (SDW) and superconducting order is a central topic in current research on the FeAs-based high Tc superconductors. Conflicting results exist in the FeAs(111) class of materials, for which whether the SDW and superconductivity are mutually exclusive or they can coexist has not been settled. Here we show that for the (Ba$_1$K$_2$)Fe$_2$As$_2$ system, the SDW and superconductivity can coexist in an extended range of compositions. The availability of single crystalline samples and high levels of energy gaps would make the materials a model system to investigate the high Tc ferropnictide superconductivity. [arXiv:0807.3950 (2008)]

1Work at APS/ANL was supported by U.S. DOE/OS/BES, under Contract No. DE-AC02-06CH11357; at USTC by National Science Foundation of China & Ministry of Science and Technology of China & National Basic Research Program of china; at LANL by U.S. DOE/OS.

1:15PM J35.00011 High magnetic field vortex torque magnetometry in SmFeAsO$_{0.8}$F$_{0.2}$ single crystals, LUIS BALICAS, ALEX GUREVICH, YOUNJUNG JO, JAN JAROSZYNSKI, DAVID LABALESTIER, National High Magnetic Field Laboratory, Florida State University, Tallahassee-FL 32310, USA, R.H. LIU, H. CHEN, XIANHUI H. CHEN, Hefei National Laboratory for Physical Science a Microscale and Department of Physics, University Science and Technology of China, Hefei, Anhui, N.D. ZHIGADOLO, S. KATRYCH, Z. BUKOWSKI, J. KARPINSKI, Laboratory for Solid State Physics, ETH Zürich, CH-8093 Zürich, Switzerland — To probe manifestations of multiband superconductivity in oxypnictides, we measured the angular dependence of magnetic torque τ(θ) in the mixed state of SmO$_{0.8}$F$_{0.2}$FeAs single crystals as functions of temperature T and high magnetic field H up to 30 T. We show that the effective mass anisotropy parameter γ extracted from τ(θ), can be greatly overestimated if the strong paramagnetism of Sm or Fe ions is not properly taken into account. The correctly extracted γ depends on both T and H, saturating at γ ≃ 9 at lower temperatures. Neither the London penetration depth nor the superfluid density is affected by high fields up to the upper critical field. Our results indicate two strongly-coupled superconducting gaps of nearly equal magnitudes.

1:27PM J35.00012 Inelastic Neutron Scattering from Fe Pnictide Superconductors, ANDREW CHRISTIANSON, Oak Ridge National Laboratory — We present inelastic neutron scattering data from both single crystal and polycrystalline specimens of several of the new Fe-based superconducting materials. The phonon density of states (PDOS) was determined for LaFeAsO$_{1-x}$F$_x$. The PDOS for the nonsuperconducting parent compound LaFeAsO was found to be nearly identical to that of superconducting LaFeAsO$_{0.8}$F$_{0.2}$. Good agreement was found between first principal calculations and the experimentally determined PDOS with the exception of a small difference in some of the Fe mode frequencies. The experimental PDOS is not consistent with conventional phonon mediated superconductivity. In the case of Ba$_2$(Fe$_{1−$x}Co$_x$)$_2$As$_2$, a magnetic excitation appears below Tc that is not present at any temperature in the parent compound Ba$_2$Fe$_2$As$_2$. The excitation occurs at an energy of 14 meV and at a wave vector consistent with antiferromagnetic correlations in the FeAs plane. The existence of this excitation is strong evidence for an unconventional superconducting gap symmetry and demonstrates that the superconducting order parameter is strongly coupled to magnetic degrees of freedom in the Fe-based superconductors.

This work was supported by the Office of Basic Energy Sciences US DOE

Tuesday, March 17, 2009 11:15AM - 2:15PM Session J36 DCMP: Si and Ge Nanowires: Electrical Transport and Simulation 408
11:15AM J36.00001 Epitaxial growth of Ge-Si,Ge$_{1-x}$ core-shell nanowire heterostructures with tunable shell content. KAMRAN VARAHRIAMYAN, DOMINGO FERRERE, EMANUEL TUTUC, SANJAY BANERJEE. The University of Texas at Austin — Core-shell nanowire heterostructures are an interesting testbed for band engineering at the nanoscale. Here we present the growth of germanium (Ge) – silicon-germanium (Si,Ge$_{1-x}$) epitaxial core-shell nanowire (NW) heterostructures, with tunable Si and Ge shell content. The Ge NWs were grown using the Au-catalyzed vapor-liquid-solid (VLS) growth mechanism. Subsequently, the Si,Ge$_{1-x}$ shells are grown in-situ, conformal onto the Ge NW using ultra-high-vacuum chemical vapor deposition. We use transmission electron microscopy to confirm that both the core and shell are single crystal, and cross-sectional transmission electron microscopy energy dispersive x-ray spectroscopy to determine the shell thickness and content. Our data show that the Si and Ge shell content can be tuned depending on the SiH$_4$ and GeH$_4$ partial pressures during the shell growth, effectively enabling band engineered core-shell nanowire heterostructures.

11:27AM J36.00002 The Effects of Strain and Quantum Confinement on the Electronic Properties of Germanium Nanowires$^1$. PAUL LOGAN, Arizona State University, XIHONG PENG, Arizona State University — Germanium nanowires are expected to play an important role as both interconnects and functional components in future nanoscale electronic and optical devices, such as light-emitting diodes, field-effect transistors, chemical and biological sensors. The study of quantum confinement on the band gap of Ge nanowires has been addressed both using theoretical methods and experimental techniques. In the present work, using first principles density-functional theory we studied the uniaxial strain effects on the electronic properties in Ge wires along [110] direction with lateral diameter up to 5 nm. Ge [110] nanowires demonstrate a direct band gap, in contrast to the nature of indirect band gap in bulk. We discovered that the uniaxial strain modulates the band gap of Ge nanowires: compressive strain increases the gap while tensile strain reduces the gap. In addition, the strain also modifies the effective masses of the electron and the hole of Ge wires. Expansion increases the effective mass of the hole, while compression increases the effective mass of the electron. Our results suggest both strain and size can be used to tune the band structure of nanowires, which may help in design of future nanoelectronic devices.

$^1$Prof. Jeff Drucker and his research group are acknowledged for experimental data.

11:39AM J36.00003 Atomic scale structure of Si nanowire. TAO XU, JEAN PHILIPPE NYS, MAXIME BERTHE, BRUNO GRANDDidier, DIDIER STEVENARD, Institut d’Electronique, de Microélectronique et de Nanotechnologie, WANGHUA CHEN, RODRIGUE LARDE, EMMANUEL CADEL, PHILIPPE PAREIGE, University and INSA of Rouen — In this work, we have succeeded to observe the atomic structures of Au assisted Vapor-liquid-solid grown Si nanowire facetten sidewalls by scanning tunnelling microscopy (STM) at low temperature. By combining transmission microscopy observations with STM measurements, we were able to identify the different facets along the growth direction of the nanowires. For nanowires with diameters larger than 150 nm, the facets orientation alternates between the [111] and [113] directions, whereas for smaller diameters, the [113] facets are replaced by facets with an orientations making a larger angle with the [111] direction. Imaging the facets at the atomic resolution clearly revealed that the facet reconstructions are induced by Au atoms. From the spectroscopic measurements, the facets are found to be metallic. In order to obtain the impurity distribution below the surface, 3D atom probe tomography analyses were performed. A uniform distribution of Boron impurities is observed in the core of the nanowire and the impurity concentration agrees well with the ratio of the flow rates between silane and diborane. Finally, such results are compared to the conductivities of single nanowires measured in field effect transistor devices.

11:51AM J36.00004 Structural and Electronic Properties of Boron Doped Multiply Twinned Silicon Nanowires. C.S. JAYANTHI, PAUL TANDY, M. YU, S.Y. WU, University of Louisville, Y. ZHAO, NREL, UNIVERSITY OF LOUISVILLE/NATIONAL RENEWABLE ENERGY LAB COLLABORATION — Previous studies of undoped multiply twinned (MT) silicon nanowires (SiNWs) have found these structures to be more stable than the bulk-cut single crystal SiNWs for diameters < 6 nm$^1$. The five segments that form the MT-SiNWs result in a strain field, causing the interior region of the MT-SiNW to compress while stretching its exterior. In fact, the distribution of the internal stress field in MT-SiNWs offers a unique opportunity for doping the MT-SiNW, including bi-polar doping, and thus opening doors to novel designs of photovoltaic elements. In this work, we will use highly efficient quantum mechanical simulations based on the semi-empirical Hamiltonian developed in Ref.$^2$ to investigate the electronic structure of boron doped MT-SiNWs of different diameters. We will first determine the most favorable locations for placing boron atoms by mapping uniaxial strain effects on the electronic properties in Ge wires along [110] direction with lateral diameter up to 5 nm. Ge [110] nanowires demonstrate a direct band gap, in contrast to the nature of indirect band gap in bulk. We discovered that the uniaxial strain modulates the band gap of Ge nanowires: compressive strain increases the gap while tensile strain reduces the gap. In addition, the strain also modifies the effective masses of the electron and the hole of Ge wires. Expansion increases the effective mass of the hole, while compression increases the effective mass of the electron. Our results suggest both strain and size can be used to tune the band structure of nanowires, which may help in design of future nanoelectronic devices.


12:03PM J36.00005 Nanometer-resolution studies of “end-on” metal contacts to vertical Si nanowires. W. CAI, Y.L. CHE, J.P. PELZ, The Ohio State Univ., E. HEMESATH, L.J. LAUHON, Northwestern Univ. — There is great interest in semiconducting nanowires (NWs) and carbon nanotubes (NTs) for future electronic devices and fundamental studies of low-dimensional systems. However, the critical contacts to NWs and NTs are still poorly understood. For example, it is predicted (but not yet demonstrated) that Fermi level pinning should be much weaker at small “end-on” NWs or NT Schottky contacts.$^1$ We have previously used cross-sectional ballistic electron emission microscopy (BEEEM) to quantify small-size effects in Schottky contacts to cleaved quantum wells.$^2$ Here we describe on-going work to study individual end-on contacts to Si NWs. Vertical Si NWs were grown on Si(111) substrates, embedded in spin-on-glass, and planarized with a chemical mechanical polish. A brief HF etch and thin Au film deposition were then used to make end-on NW contacts. Initial studies with AFM, SEM, internal photoemission spectroscopy, and BEEEM demonstrate we can make and measure end-on Schottky contacts to 80nm diameter Si NWs. We will discuss on-going work to optimize sample processing (to reduce roughness near the NWs) and then to quantify the dependence of local contact properties on Si NW diameter. Work supported by NSF Grant No. DMR-0805237.$^1$ F. Leonard et al., Phys. Rev. Lett. 84, 4693 (2000).$^2$ C. Tivarus et al., Phys. Rev. Lett. 94, 206803 (2005).

12:15PM J36.00006 First-Principles Simulations of Silicon Nanowires with Different Surface Passivations. JUNWEN LI, JOHN W. MINTMIRE, Department of Physics, Oklahoma State University — We report first-principles simulation results for the electronic band structure of silicon nanowires along $<$100$>$ and $<$110$>$ directions with different surface passivating groups such as hydrogen, hydroxyl, and methyl within an all-electron, Gaussian type orbital, local density functional approach. We discuss how these different groups affect the band gaps and electron distribution of silicon nanowires. And from the band structures we find that the carrier effective masses of $<$100$>$-oriented silicon nanowires exhibit much more dependence on the diameter and passivation compared to those of $<$110$>$-oriented nanowires.$^1$ This work was supported by the US Department of Energy Grant DE-FG02-07ER46362.

$^1$This work was supported by the US Department of Energy Grant DE-FG02-07ER46362.
12:27PM J36.00007 Study of Electronic Charge Distribution in Silicon Nanowire Transistors: An Atomistic Approach\(^1\), ABHIJEEET PAUL, SAUMITRA MEHROTRA, GERHARD KLIMECK, Purdue University — Atomistic modeling has been performed to investigate the spatial electronic charge distribution in silicon nanowire cross-sections. The modeling approach involves solution of electronic bandstructure using the 20 band sp\(^{3d5s*}\)-SO nearest neighbor Tight-binding (TB) method with spin orbit (SO) interaction (LCAO) solved self-consistently with a two dimensional Poisson equation. Nanowires with rectangular, circular and triangular cross-section shapes have been investigated, with cross-section size of 3.1 nm and 5.1 nm for three different crystal orientations namely [100], [110] and [111]. The observed charge distribution as observed in these wires, is a strong function of cross-section shape, size and crystal orientation. [100] and [110] wires show strong corner effects, however, [111] oriented wires have centralized charge distribution. Charge distribution is sensitive to the structural and crystal symmetry of the nanowire. Structural confinement breaks the symmetry that manifests in the 1D energy dispersion of these wires by lifting up the degeneracy at the gamma valley. Finally, we enable the understanding of atomistic treatment for charge distribution in the capacitance measurements in these ultra-scaled silicon nanowire transistors.

\(^1\)Computational resources from NCN, nanoHUB has been used. Also SRC and NSF funding has been provided to the authors.

12:39PM J36.00008 Interface State Disorder Dominated Microwave Conductance in Silicon Nanowires, CLARK HIGHSTRETRE, MARK LEE, Sandia National Laboratories, DAVID H. DUNLAP, University of New Mexico, AARON L. VALLETT, SARAH M. EICHELF, JOAN M. REDWING, THERESA S. MAYER, The Pennsylvania State University — We have developed a technique to measure the microwave conductance spectra of nanostructures at frequencies from 100 MHz to 50 GHz and at temperatures between 4 K and 300 K. We have used this technique to measure the microwave conductance spectra of doped silicon nanowires (SiNWs) which are found to increase sublinearly with frequency as \( f^{-0.5} \) to \( f^{-0.45} \), indicative of disordered conduction. Additionally, the exponents are found to be nearly independent of temperature suggesting that structural disorder in nanowire morphology, rather than energetic trapping, dominates the AC transport. A model was developed that explains the SiNW conductance in terms of carrier confinement in a disordered electrostatic potential caused by charged Si/SiO\(_2\) interface states. These results highlight the importance of topological effects in the microwave properties of nanomaterials. Results from the measurement of other nanomaterials will also be briefly presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

12:51PM J36.00009 Effect of hydrogen passivation on the structure and energetics of silicon nanowires, ABRAHAM AHMIEL, YONGQIANG XUE, SUNY Albany — In this work we explore systematically the structure, energetics and electronic properties of silicon nanowires (SiNWs) with different surface structures and growth directions, and the trend of such property variation with increasing nanowire diameters using first principles density functional theory with both local atomic basis and plane waves. Both passivated and unpassivated systems were studied. The unpassivated (100) and (111) wires are found to be metallic with the unpaired electrons on the surface of these wires acting as conducting channels. Hydrogen passivation of these surfaces introduces a direct band gap by confining the electrons to localized bonds. The nature of the electronic states is examined through local density of states and electron density distributions. The relative stability of SiNWs with different growth directions and surface structures are evaluated from the free energy of formation.

1:03PM J36.00010 Semiconducting nanowire devices in out-of-plane geometry, PRADEEP MANANDHAR, SAMUEL T. PICRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Semiconducting nanowires are attractive components in the field of nanoelectronics, photonic and sensing applications. Experiments with nanowires have usually been performed in planar geometry. Here, we demonstrate the fabrication of nanowire devices in out-of-plane geometry by taking advantage of inherent growth direction of nanowire using the vapor-liquid-solid (VLS) method. Highly epitaxial semiconducting nanowires are grown on doped Si (111) substrate from Au nanoparticle seeds assembled in e-beam lithography patterns. The directed assembly of Au nanoparticles is achieved by molecular recognition through silanization process, or electrophoretic assembly. The versatility of the VLS method allows the growth of a wide range of semiconducting nanowires with controlled in-situ doping. The post-growth processes include CVD of SiO\(_2\) filler layer, chemical mechanical polishing and light etching of the SiO\(_2\) layer to expose nanowire tips. Top metal contacts are then deposited for electrical characterization and sensing applications. We will present the results of the vertical nanowire device performance.

1:15PM J36.00011 Top-gate Ge\(_{1-x}\)Si\(_x\)Ge\(_{1-y}\) core-shell nanowire field effect transistors with highly doped source and drain,\(^1\) JUNGHYO NAH, E.-S. LIU, D. SHAHRJERDI, K. M. VARAHRAMYAN, S. K. BANERJEE, E. TUTUC, University of Texas at Austin — Semiconductor nanowires (NWs) field effect transistors (FETs) have been considered as candidates for aggressively scaled complementary metal-oxide-semiconductor (CMOS) devices. In particular, germanium (Ge) NW have been of interest thanks to their higher carrier mobility, compared to silicon (Si). Most of the reported semiconductor NW FETs to date are measured on devices with metal (Schottky) contacts, where the carrier injection efficiency into the channel is significantly limited by the Schottky barrier at the metal/NW interface. Using low (3keV) energy boron ion implantation, we demonstrate here top-gate Ge\(_{1-x}\)Si\(_x\)Ge\(_{1-y}\) core-shell NW p-type FETs, with highly doped source (S) and drain (D). The highly doped, up to \(10^{20}\) cm\(^{-3}\) levels, S/D regions of the NW FETs allow an efficient carrier injection into the NW and a low contact resistance. Compared to similar top gated NW FETs, but with undoped S/D and with metal-semiconductor contacts, the electrical characteristics of the top-gated NW FETs with doped S/D exhibit up to two orders of magnitude higher current, and an improved ON/OFF current ratio.

\(^1\)This work was funded by DARPA contracts HR0011-08-1-0050 and N66001-07-12013, and by NRI-SWAN.

1:27PM J36.00012 Precision transport and assembly of nanowires in suspension by electric fields, D.L. FAN, ROBERT CAMMARATA, C.L. CHIEN, Johns Hopkins University. MATERIALS TEAM, PHYSICS TEAM — We describe a method of precision transport of nanowires in suspension using a combination of dielectrophoretic force and electrophoretic force, which, respectively, aligns and transports the nanowires. We revealed the effect of electroosmosis flows on the nanowires and determined the ratio of viscous coefficients for nanowires moving parallel or perpendicular to the orientations. The transport of nanowires can be made to follow any prescribed trajectory with any orientation by the voltages applied to the patterned electrodes. As a demonstration of the high precision of manipulation, we have joined end-to-end two oppositely charged nanowires originally separated by 200 \(\mu\)m into a microelectromechanical device.

1:39PM J36.00013 Thermal properties measurements of silicon nanowires at low temperature, HERON JEAN-SAVIN, FOURNIER THIERRY, BOURGEOS OLIVIER, Neel Institut, CNRS, Grenoble, France — Phonons transport in nanowires and nanotubes is an effervescent field for theoretician as well as experimentalist. Especially at low temperature, where the dimension of the sample approximate the dominant phonon wave length, the low dimensionality of these systems has strong impact on the thermal transport. Specific regimes have to be considered: transmission coefficient to the heat bath, quantum regime, transition between diffusive and specular regime etc. . Firstly, we have performed measurements with the 3\(\mu\)m method on various suspended silicon nanowires with a section of the order of 100\(\mu\)m and a length of 10\(\mu\)m. Above 2 K, the thermal conductance varies like \(T^{-1}\)(Casimir Regime); however at lower temperature, a quadratic regime in temperature appears: the signature of a change in the phonon transport regime. Secondly, we have measured nanowires with various geometries, to deduce the impact of geometrical factors at the mesoscopic scale on the thermal transport. All these results will be discussed in view of the different models describing the heat transfer at the nanoscale.
1:51PM J36.00014 ABSTRACT WITHDRAWN

2:03PM J36.00015 Donor-pair defects and doping efficiency in silicon nanowires , BYUNGKI RYU, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, 305-701, CHANG-YOUN MOON, Department of Physics and IPAP, Yonsei University, Seoul 120-701, WON-JIN LEE, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, 305-701 — We investigate the doping efficiency of dopants in Si nanowires through first-principles density-functional calculations. For hydrogen- passivated Si nanowires doped with group-V elements such as P, As, and Sb, we consider wire diameters in the range of 8 - 30 Å and axis orientations along the [111] and [110] directions. A single substitutional donor prefers to locate on the wire center and acts as a shallow donor. When wire diameters are below a critical value, a donor-pair defect which consists of two dopants at the first-nearest distance can be stabilized, in contrast to bulk Si. The stability of the donor-pair defect is attributed to the confinement effect in nanostructures, which results in the increase of the band gap and thereby the destabilization of the shallow donor level. As the donor-pair defect with a deep level in the band gap is electrically inactive, the doping efficiency expected to be low in small-diameter nanowires. The formation of the donor-pair defect is found to be more favorable for the P dopants, which have a smaller atomic radius than the As and Sb dopants.

Tuesday, March 17, 2009 11:15AM - 2:15PM —
Session J37 DCP: Focus Session: Spectroscopic Probes of Biomolecular Structure and Function
II 409

11:15AM J37.00001 Structures of Amyloid Fibrils and Protein Folding Intermediates: New Insights from Solid State NMR, ROBERT TYCKO, National Institutes of Health — I will present recent results from two projects: (1) We are using a combination of solid state NMR techniques and electron microscopy techniques to develop full molecular models for amyloid fibrils formed by the beta-amyloid peptide of Alzheimer’s disease and by other peptides and proteins. Amyloid fibrils are often polymorphic, so that the detailed molecular structure depends on growth conditions or other factors. I will describe two structural models for beta-amyloid fibrils with two distinct morphologies. I will also describe efforts to determine which fibril structure develops in the brains of Alzheimer’s disease patients, and solid state NMR methods that contribute to our amyloid studies; (2) Structural properties of unfolded or partially folded states of proteins are not well understood. In principle, solid state NMR measurements on freeze-dried trapped-ideal-state samples reveal idealized structures and provide access to the structural properties of proteins in the unfolded states (i.e., denatured states) and on transient states that are trapped by freezing on the microsecond time scale. Both types of experiments reveal structural properties that are unanticipated and could not be detected by more conventional protein folding measurements.

11:51AM J37.00002 Two-Dimensional Infrared Probes of Peptide Conformations: the 3α-Helical Secondary Structure, NIEN-HUI GE, Department of Chemistry, University of California, Irvine — The 3α-helix is a secondary structure that has important biological functions and has been proposed as a picosecond intermediate in the folding of α-helices. Two-dimensional infrared (2D IR) spectroscopy with its high structural sensitivity and time resolution is a powerful approach for investigating the structure and dynamics of peptides and proteins. In this talk, we will describe how we are using 2D IR and isotope labeling to study 3α-helical oligopeptides that are rich in C13-methylated amino acids. These peptides are attractive models for developing and refining new and theoretical approaches to peptide conformational analysis. By manipulating networks of vibrational modes using judicious choices of laser polarizations and pulse ordering, we demonstrate that 2D IR can provide diagnostic cross-peak patterns for distinguishing different helical structures and probe the onset of 310-helical secondary structure. Using a series of peptides with 13C=18O and 15N isotope labels, we observe cross-peak signatures that reveal vibrational couplings between amide-I and amide-II modes across a 310-helical hydrogen bond. The results provide a direct evidence for local helical structure formation. Experimental spectra are compared to simulations based on nonlinear response theory, vibrational eigenstates and couplings derived from DFT-optimized structures, and trajectories from molecular dynamics simulations.

12:27PM J37.00003 Earle K. Plyler Prize Talk: Using High Resolution Electronic Spectroscopy to Probe Reactive Chemical Intermediates, TERRY MILLER, Ohio State University — Gas phase chemical reactions, such as occur in atmospheric chemistry, combustion, plasma processing, etc. are of great importance to our economy and society. These reactions are typically very complex involving up to 1000's of elementary steps with a corresponding number of reactive chemical intermediates. Spectroscopic diagnostics, based upon well analyzed and well understood spectra of the intermediates, are crucial for monitoring such reactions and unraveling their mechanisms. These spectral analyses often benefit from the guidance provided by quantum chemical calculations and conversely the molecular parameters, experimentally determined from the spectra, serve as “gold standards” for benchmarking such calculations. Such standards are especially valuable for reactive intermediates whose electronic structures are particularly complex because of electronic-spin interactions, Jahn-Teller effects or other vibronic interactions, hindered internal motions, large molecular size and weight, etc. The organic alkoxyl, RO-, and peroxy, ROO2-, (R=alkyl group) free radicals are excellent examples of such species. The talk will focus on our recent characterization of these radicals via their “high-resolution,” mostly rotationally resolved, electronic spectra utilizing the techniques of laser induced fluorescence, stimulated emission pumping, and cavity ringdown spectroscopy. Selected spectra, their analysis, and the molecular information resulting therefrom will be discussed.

1:03PM J37.00004 Solvent induced fluctuations and the collective librational dynamics of myoglobin, hemoglobin, and lysozyme studied with infrared spectroscopy, KRISTINA WOODS, Carnegie Mellon University — We will discuss the use of [THz and Mid-] infrared spectroscopy to investigate the dynamics of several globular proteins under varying hydration and temperature conditions. Analysis of the experimental spectra has revealed that the amount of solvent in the hydration shell has a strong influence on the amplitude and the rate of relaxation associated with the low frequency protein conformational fluctuations and also the arrangement of hydrogen bonds in the protein secondary structure. At a hydration level > 0.2 we identify modes in the secondary structure of all of the proteins investigated that suggest extra mobility in the protein structure that is not present at low hydration. We will discuss how greater insight into the origin and nature of these detected solvent induced fluctuations may be important for developing a better understanding about energy localization and its relationship with biological function.

1:15PM J37.00005 Label-Free Determination of Protein Binding in Aqueous Solution using Overlayer Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (OE-ATR-FTIR), TRAVIS RUTHENBURG, TOLULOPE AWEADA, SIMON PARK, CLAUDE MEARES, DONALD LAND, Department of Chemistry, University of California, Davis — Protein binding/affinity studies are often performed using Surface Plasmon Resonance techniques that don’t produce much spectral information. Measurement of protein binding affinity using FTIR is traditionally performed using high protein concentration or deuterated solvent. By immobilizing a protein near the surface of a gold-coated germanium internal reflection element interactions can be measured between an immobilized protein and free proteins or small molecules in aqueous solution. By monitoring the on and off rates of these interactions, the dissociation constant for the system can be determined. The dissociation constant for the molecule Yttrium-DOTA binding to the antibody 2D12.5 system was determined to be 100M. Results will also be presented from our measurements of Bovine Serum Albumin (BSA) binding to anti-BSA.
1:27PM J38.00006 Solute-protein interactions: Variations in correlation times and spin label mobility. MANDY BLACKBURN, LUIS GALIANO, ANGELO VELORO, GAIL FANUCCI, University of Florida — Using EPR, NMR and fluorescence spectroscopy, the effects of several viscogen monomers (sucrose, glycerol, and ethylene glycol) and macromolecular crowding polymers (Ficoll400 and various size polyethylene glycols (PEG)) on the mobility of spin labels at aqueous exposed sites in the flap of HIV-1 protease, the correlation time of this protein, as well as conformation of the hair pin flaps were investigated. Results show that, as expected, protein correlation time is more strongly altered by the small viscogens compared to the macromolecular crowders. On the other hand, EPR line shapes reveal that the chemistry (ie hydrophobicity) and not the size of the solutes correlates to changes seen in the spectra. The conformations of the β-hair pin flaps in HIV-1 protease were unchanged by any of solutes as determined by pulsed EPR distance measurements. Thus, indicating that specific solute interactions with the surface of the protein are responsible for the changes observed in the EPR spin label spectra.

1:39PM J38.00007 On The Electronic Properties of Photoacoids In The Gas Phase. Electric Dipole Moments of CIS- and TRANS-2-Naphthal当地 M. HAMERS, J. STOKBRO, University of Pittsburgh — The permanent electric dipole moments (μ) of two conformers of 2-naphthol (2HN) in their ground and electronically excited states have been experimentally determined by Stark-effect measurements in a molecular beam. Upon UV excitation, little change in the magnitudes of μ is observed, but the orientation of the dipole moment within each conformer shifts significantly, indicating photon-induced rearrangements in electronic distributions. cis-2HN has Δμ = -0.17 D and Δθ = -28° and trans-2HN has Δμ = 0.05 D and Δθ = +28° (trans-2HN). The Δθ values for the two conformers differ in sign. The small changes in the magnitudes of the dipole moments suggest that the isolated molecules do not undergo large charge separations upon excitation. Our study, void of solvent perturbations, is of importance to the larger community currently describing aromatic biomolecule and “super” photoacoid behavior via theoretical modeling and condensed phase solvatocromism.

1:51PM J38.00008 Threading of Binuclear Ruthenium Complex Through DNA Bases THAYA-PARAN PARAMANATHAN, Department of Physics, Northeastern University, Boston, MA, USA., FREDRIK WESTERLUND, Nano-Science Center, University of Copenhagen, Copenhagen, Denmark., MICAIA MCCAULEY, Department of Chemistry, Northeastern University, Boston, MA, USA., PER LINCOLN, Department of Chemical and Biological Engineering, Chalmers University of Technology, Goteborg, Sweden., IOULLA ROUZINA, Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN, USA., MARK WILLIAMS, Department of Physics, Northeastern University, Boston, MA, USA. — Due to steric constraints the dumb-bell shaped binuclear ruthenium complex can only intercalate DNA by threading, which requires local melting of the DNA to occur. By mechanically manipulating a single DNA molecule held with optical tweezers, we lower the barrier to threading compared to bulk experiments. Stretching single DNA molecules with different drug concentrations and holding a constant force allows the binding to reach equilibrium. We can obtain the equilibrium fractional ligand binding and length of DNA at saturation. Fitting these results yields quantitative measurements of the binding thermodynamics and kinetics. In addition, we obtain the minimum binding site size, which may be determined by either electrostatic repulsion or steric constraints.

2:03PM J38.00009 Raman Spectral Signatures as Conformational Probes of Biomolecules1. ILANA BAR, AMIR GOLAN, NITZAN MAYORKAS, SALMAN ROSENWAKS, Ben Gurion University of the Negev — A first application of ionization-loss stimulated Raman spectroscopy (ILSRS) monitoring the spectral signatures of four conformers of a gas phase neurotransmitter (2-phenylethylamine) is reported. The Raman spectra of the conformers show bands that uniquely identify the conformational structure of the molecule and are well matched by density functional theory calculations. The measurement of spectral signatures by ILSRS in an extended spectral range, with a relatively convenient laser source, is extremely important, allowing enhanced accessibility to intra- and inter-molecular forces, which are significant in biological structure and activity.

Session J38 DCP: Focus Session: Theory of Electron Transport Through Molecules II

11:15AM J38.00001 Transport in Molecular Junctions: Thoughts Coherent and Incoherent . MARK RATNER, Northwestern University — Current experimental efforts are clarifying quite beautifully the nature of charge transport in so-called molecular junctions, in which a single molecule provides the channel for current flow between two electrodes. The theoretical modeling of such structures is challenging, because of the uncertainty of geometry, the nonequilibrium nature of the process, and the variety of available mechanisms. The talk will center on the formulation of the problem in terms of non-equilibrium theory, and then on the generalizations needed to make that simple picture relevant to the real experimental situation. These include antiresonances, vibronic coupling and its control, structural disorder and representations for the electronic structure. Comments will be made on the measurements of inelastic spectra, and the information to be gained from them.

11:51AM J38.00002 Theoretical aspects of modeling the conductance of molecular junctions . KURT STOKBRO, QuantumWise A/S — In this talk I will discuss different semi-empirical and ab initio approaches for modeling the coherent electron transport of molecular junctions using the non-equilibrium Greens function formalism [1]. The most important effects for determining the conductance are the energies and coupling of the frontier molecular orbitals to the electrodes. I will discuss the accuracy of different levels of theory for calculating the HOMO-LUMO gap of various molecules, and present a simple correction that improves the accuracy of Density Functional based mean field theories [2]. The physical origin of the correction is illustrated using the Moshinsky atom as test system, and the accuracy is illustrated for a number of small molecules [3]. The coupling of the molecule to the electrodes is controlled by the terminal group on the molecule. We illustrate how a molecule with C60 terminal groups can have a very strong coupling with the electrodes [4].

12:27PM J38.00003 ABSTRACT WITHDRAWN

1Work supported by NSF (CHE-0615755).
12:39PM J38.00004 Many-body theory of electron transport in single-molecule junctions. CHARLES STAFFORD, JUSTIN BERFIELD, University of Arizona — Currently, there is no general theory to treat the many-body problem of a single molecule coupled to metallic electrodes. Mean-field approaches such as density-functional theory—the dominant paradigm in quantum chemistry—have serious shortcomings because they do not account for important interaction effects like Coulomb blockade. We develop a systematic theoretical framework for this nonequilibrium many-body problem, starting from an exact diagonalization of the few-body problem of an isolated molecule, and including lead-molecule coupling perturbatively in a novel application of nonequilibrium Green’s functions.

12:51PM J38.00005 Quantum theory of image potential and resonant tunneling in molecular junctions. LUDUMYLA ADAMSKA, IVAN OLEYNIK, University of South Florida, MORTIKO KOZHUSHNER, Institute of Chemical Physics, Russian Academy of Sciences, Russia — It has recently been realized that the image potential plays an important role in charge transport through single organic molecules. In most cases, the classical image potential -1/4z is used to calculate the modified energy spectrum of the charge carriers in the molecule. In this talk, we will present the theory of resonant tunneling transitions that include the quantum mechanical effects of dynamic image potential due to the polarization interaction of the tunneling charge carrier (electron or hole) with surface plasmons. The application of this theory to organic molecular junctions of experimental interest will be discussed.

1:03PM J38.00006 Charge and Spin Memory Effects in Molecular Junctions1, P. D’AMICO, D.A. RYNDYK, Regensburg Uni, G. CUNIBERTI, T.U. Dresden, K. RICHTER, Regensburg Uni — In the field of molecular electronics, effects like charge-memory, bistability and switching between charged and neutral states have been observed in STM [1] and single-molecule junctions [2] experiments. In this work we use model Hamiltonians to describe molecular junctions, including electron-electron and electron-vibron interactions as well as tunneling coupling to the leads. For a molecular level coupled to a vibron and in the presence of leads, we show that upon applying gate or bias voltage, it is possible to observe charge-bistability and hysteretic behavior. Physical quantities like lifetimes, charge-voltage and current-voltage curves are calculated by the master equation method for weak coupling to the leads [3] and at stronger coupling by the equation-of-motion method for noneq. Green functions, performing a systematic analysis of the bistable behaviour of the system for different internal parameters such as the electron-vibron and the lead-molecule coupling [4]. In the case of a spin-degenerate level in a single and double dot molecule with vibrational coupling and in presence of ferromagnetic leads, we consider the possibility to obtain a spin-memory effect. [1] J.Repp et al, Science 305, 493 (04); [2] E.Lortscher et al, Small 2, 973 (06); [3] D.A.Ryndyk et al, PRB 78, 085409 (08); [4] P.D’Amico et al, NJP 10, 085002 (08).

1We acknowledge support from the DFG project “Quantum Transport from the Molecular Scale.”

1:15PM J38.00007 A simple model for the description of correlation effects in molecular conductors1, MATTHIAS ERNZERHOF, FRANCOIS GOYER, Department of Chemistry, University of Montreal — To model transport through molecular electronic devices (MDEs), we use a non-Hermitian Hamiltonian [1] for the description of open systems that exchange current density with their environment. The infinite contacts are replaced by complex source-sink potentials (SSPs) [1]. Employing a Hubbard interaction term, we include electron-correlation effects in our approach [2]. Electron interaction is considered in the molecule and neglected in the contacts. Among other strongly correlated problems, we discuss the change in conductance upon bond breaking. In the limit where the electron repulsion is strong compared to the binding energy (as it is the case in a stretched bond) a strong suppression of conductance is observed due to the localization of electrons. Other interesting phenomena, which cannot be accounted for with conventional (independent electron) approaches, are discussed as well. [1] F. Goyer, M. Ernzerhof, and M. Zhuang, J. Chem. Phys. 126, 144104 (2007); [2] M. Ernzerhof, J. Chem. Phys. 127, 204709 (2007). [2] A. Goker, F. Goyer, and M. Ernzerhof, J. Chem. Phys. 129, 194901 (2008); M. Ernzerhof, J. Chem. Phys. 125, 124104 (2006).

1We gratefully acknowledge financial support provided by NSERC.

1:27PM J38.00008 Effects of dephasing on molecular conduction1, JESSE MAASSEN, FERDOWS ZAHID, HONG GUO, Centre for the Physics of Materials and Department of Physics, McGill University, Montreal, Canada — In this work, we theoretically investigate effects of dephasing on electron transport in molecular wires. The quantum transport analysis is carried out using the density functional theory (DFT) combined with the non-equilibrium Green’s function framework (NEGF). The dephasing effect is included at a phenomenological level by introducing fictitious voltage probes to the NEGF-DFT formalism that mimics the randomisation of quantum phase information of the charge carriers. For three systems: (i) a 1,4-benzenedithiol (BDT) molecule connected to Al(001) leads; (ii) an atomic gold chain in contact with Au(001) leads; and (iii) a very narrow Al(001) nanowire, our results indicate that there are two behaviours. When the wires are not conductive as (i,ii), the dephasing effects can increase conduction for a range of system parameters; while for (iii) the dephasing on electron transport in molecular wires. The quantum transport analysis is carried out using the density functional theory (DFT) combined with the non-equilibrium Green’s function framework (NEGF). The dephasing effect is included at a phenomenological level by introducing fictitious voltage probes to the NEGF-DFT formalism that mimics the randomisation of quantum phase information of the charge carriers. For three systems: (i) a 1,4-benzenedithiol (BDT) molecule connected to Al(001) leads; (ii) an atomic gold chain in contact with Au(001) leads; and (iii) a very narrow Al(001) nanowire, our results indicate that there are two behaviours. When the wires are not conductive as (i,ii), the dephasing effects can increase conduction for a range of system parameters; while for (iii) the dephasing effect is small. These effects can increase conduction for a range of system parameters; while for (iii) the dephasing effect is small. These effects can increase conduction for a range of system parameters; while for (iii) it is comparable to the case of a perfectly conductive wire.

1The authors acknowledge support from the FQRNT, NSERC and CIFAR.

Tuesday, March 17, 2009 11:15AM - 2:03PM — Session J39 DBP: Lipid Bilayers: Structure and Function II 411

11:15AM J39.00001 Membrane curvature sensitively by the actin cytoskeleton. GHEE HWEE LAI, ABHUJIT MISHRA, NATHAN SCHMIDT, University of Illinois at Urbana-Champaign, DANIEL KAMEI, TIMOTHY DEMING, University of California, Los Angeles, GERARD C. L. WONG, University of Illinois at Urbana-Champaign — Biological active molecules such as proteins and oligonucleotides can be transduced across cell membranes with high efficiency by cell penetrating peptides. It has been recently demonstrated using synchrotron x-ray diffraction that such peptides induce saddle-splay (negative Gaussian) membrane curvature, which is the topological requirement for pore formation. Here, we show how the actin cytoskeleton ‘senses’ and responds to negative Gaussian defects on a membrane, by examining the interaction between cell penetrating peptides and an active polymerizing cytoskeleton encapsulated within giant unilamellar vesicles, and compare the results to cell based studies.

11:27AM J39.00002 Optically Induced Rotation of Laser-trapped Chiral Lipid Tubules by Linearly Polarized Light. NATTAPORN CHATTHAM, THANATE NA WICHAN, APICHART PATTANAPORKRATANA, JANMRAS LIMTRAKUL, Kasetsart University, KASETSART UNIVERSITY TEAM — Chiral Phospholipids are found self-assembled into fascinating cylindrical tubules of 500 nm in diameter by helical winding of bilayer stripes under cooling in ethanol and water solution. Theoretical prediction and experimental evidence reported so far confirmed the modulated tilt direction in a helical striped pattern of the tubules. This molecular orientation morphology results in optically birefringent tubules. We investigate them under optical trap of 532 nm linearly polarized optical tweezers. We observed spontaneous rotation of lipid tubules induced by radiation torque. The tubule direction can be controlled by the alignment of polarization direction, and thus the rotation angle can be specified. Other related aspect on optical activity of the lipid tubules is also studied. This work is supported by Kasetsart University Research and Development and National Nanotechnology Center, Thailand.
and revealed a good agreement with the FTIR and Raman spectroscopic results. Synthetic lipids with a hydrophilic oligomer covalently coupled to the substrate serve as membrane anchors while forming a nm-thick aqueous reservoir. This property can be exploited to investigate protein-membrane interactions at the molecular length scale. The anchor is chemisorbed to a self-assembled monolayer, either as a pure compound (densely tethered) or laterally diluted (sparingly tethered) by β-mercaptoethanol (β-ME), a small spacer. Phospholipids are then precipitated to complete the bilayer structure. Diffusion measurements were performed using both one-photon and two-photon fluorescence correlation spectroscopy using the Z-Scan approach[2]. While the aqueous reservoir decouples the bilayer from the substrate, we expect the presence of tethers in the inner leaflet to inhibit the free diffusion of lipids. Indeed, we see a drop in the apparent diffusion coefficient by a factor of 2 when comparing a densely tethered membrane to a sparsely-tethered membrane. Importantly, the diffusion coefficients in tBLMs compare favorably with those observed in giant unilamellar vesicles, indicating that tBLM dynamics are similar to those of free bilayers. [1] McGillivray et al., Biointerphases 2007(2): 21–33 [2] Benda et al., Langmuir 2003(19): 4120-4126.

**11:51AM J39.00004 Cholesterol Perturbs Lipid Bilayers Non-Universally**¹, JOHN NAGLE, JIANJUN PAN, THALIA MILLS, STEPHANIE TRISTRAM-NAGLE, Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213 — Cholesterol is well known to modulate the physical properties of biomembranes. Using modern X-ray scattering methods, we have studied the effects of cholesterol on the bending modulus Kc, the thickness Dhm, and the orientational order parameter Szz of lipid bilayers. We find that the effects are different for at least three classes of phospholipids characterized by different numbers of saturated hydrocarbon chains. Most strikingly, cholesterol strongly increases Kc when both chains of the phospholipid are fully saturated but not at all when there are two mono-unsaturated chains.

¹This research was supported by NIH Grant GM 44976. Synchrotron beam time was provided by CHESS, which is funded by NSF Grant DMR-0225180.

**12:03PM J39.00005 Barrier Function of Lipid Membrane in the Interaction with Nanostructures**, SERGIY MINKO, Clarkson University, YURY ROITER — Tiny details of the phospholipid (DMPC) membrane morphology in close vicinity to nanostructured silica surfaces have been discovered in the atomic force microscopy experiments. The structural features of the silica surface were varied in the experiments by the deposition of silica nanoparticles of different diameter on plane and smooth silica substrates. It was found that, due to the barrier function of the lipid membrane; only particles larger than 22 nm in diameter, with a smooth surface were completely enveloped by the lipid membrane. However, nanoparticles with bumpy surfaces (curvature diameter of bumps that as that of particles <22 nm) were only partially enveloped by the lipid bilayer. For the range of nanostructure dimensions between 1.2 nm and 22 nm, the lipid membrane underwent structural rearrangements by forming pores (holes). The nanoparticles were accommodated into the pores but not enveloped by the lipid bilayer. The study also found that the lipid membrane conformed to the substrate with surface structures of dimensions less than 1.2 nm without losing the membrane integrity.

**12:15PM J39.00006 Direct nm-scale observation of lipid membrane fluctuations**, SUNG CHUL BAE, YAN YU, Department of Materials Science and Engineering, University of Illinois, STEPHEN M. ANTHONY, Department of Chemistry, University of Illinois, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois — Thermal fluctuation of giant unilamellar phospholipid vesicles (GUVs) was observed by a combination of direct imaging using epifluorescence microscopy and forward laser beam scattering of a laser beam from the vesicle edge. The latter technique allows for the quantitative measurement of lipid membrane fluctuations due to the presence of rafts. Using high performance microscopy and a specialized data analysis scheme, we were able to extract information about lipid membrane fluctuations at nanometer length scales over a range of temperatures. These results are consistent with previous lipid dynamics experiments, and provide a valuable tool for understanding membrane structure and function.

**12:27PM J39.00007 Effects of mobile membrane proteins on the structure and dynamics of lipid rafts**, JUN FAN, MARIA SAMMALKORPI, Mechanical and Aerospace Engineering, MIKKO HAATAJA, Mechanical and Aerospace Engineering, Princeton Institute for the Science and Technology of Materials, Program in Applied and Computational Mathematics — Compositional lipid domains (“lipid rafts”), which reside in the plasma membrane, are thought to facilitate many important cellular processes, including signal transduction and viral entry. Experimentally, raft dynamics have been probed mainly indirectly through observations of raft-associated membrane proteins, and the interpretation of the data relies heavily on assumptions about raft shape and viscosity. Previously, we have shown that strong interactions between rafts and immobile protein clusters may induce the formation of spatially extended raft aggregates [J. Fan et al., PRL 100, 178102 (2008)], thus complicating the interpretation of experimental data. In this work, we present a novel model that explicates the dynamics of membrane proteins with the underlying time-dependent raft domain structure via a hybrid continuum-particle simulation scheme, and develop strategies for extracting quantitative information about raft dynamics from observations of the membrane proteins alone.

**12:39PM J39.00008 Multiscale Modeling of supported bilayers**, ROLAND FALLER, CHENYUE XING, MATTHEW I. HOOPES, UC Davis — Supported Lipid Bilayers are an abundant research platform for understanding the behavior of real cell membranes as they allow for additional mechanical stability. We studied systematically the changes that a support induces on a phospholipid bilayer using the coarse-grained Martini model. It turns out that there is at equilibrium about a 2-3% higher density in the proximal leaflet. These results are in favorable agreement with recent data obtained by very large scale modeling using a water free model where flip-flop can be observed directly. We compare results of the free energy of transfer obtained by pulling the lipid across the membrane in different ways. There are small quantitative differences but the overall picture is consistent. We are additionally characterizing the intermediate states which determine the barrier height and therefore the rate of translocation.

**12:51PM J39.00009 Thermotrophic vibrational spectroscopy of newly developed self-forming PEGylated lipids**, RAJAN BISTA, REINHARD BRUCH, AARON COVINGTON, University of Nevada, Reno, Nevada, USA — Vibrational spectroscopy can provide valuable structural information about lipids, which are important molecular components of biological membranes. In the present study, we have focused on the thermotropic vibrational spectroscopy of two newly developed synthetic PEGylated lipids trademarked as QuSomes to investigate the phase behaviors and associated changes in the conformational order. In contrast to conventional phospholipids, this new kind of lipid forms liposomes spontaneously upon hydration, without the supply of external activation energy. Variable-temperature thin-layered Fourier Transform Infrared (FTIR) spectroscopy and Raman spectroscopy have been developed and employed in order to plot the transition temperature profiles showing the phase behavior of these new lipids composed of 1,2-dimyristoyl-rac-glycerol-3-dodecylamine glycol (GDM-12) and 1,2-distearyl-rac-glycerol-3-tricosylamine glycol (GGS-23). Furthermore, several spectral indicators were calculated and correlated which allowed for the deduction of various aspects of molecular structure as well as intramolecular motion and intermolecular interactions occurred during temperature change. To confirm the observations, differential scanning calorimetry (DSC) was applied and revealed a good agreement with the FTIR and Raman spectroscopic results.
The results elucidate the mechanism by which PG-1 uses to induce leakage in bacterial cells. The structural transformation can be understood in the framework of the action of 1d detergent, with PG-1 acting as a line in model membranes via atomic force microscopy for the first time. PG-1 induces structural transformations in supported lipid bilayers, progressing from bilayer separation of charged and neutral lipid molecules in mixed lipid monolayers, and discuss the dependence on pH, salt concentration and ion valency.

To study the mechanism of action of PG-1, we directly visualize the topological changes induced by PG-1 forming pores which increase membrane permeability to ions or larger molecules. It has been proposed that PG-1 selectively induces stable membrane pores in bacterial membranes over mammalian membranes. To investigate the mechanism of action of PG-1, we directly visualize the topological changes induced by PG-1.

1:03PM J39.00010 Theory of Disk-to-Vesicle Transformation, Jianfeng Li, An-Chang Shi, Department of Physics and Astronomy, McMaster University — Self-assembled membranes from amphiphilic molecules, such as lipids and block copolymers, can assume a variety of morphologies dictated by energy minimization of system. The membrane energy is characterized by a bending modulus ($\kappa$), a Gaussian modulus ($\kappa_G$), and the line tension ($\gamma$) of the edge. Two basic morphologies of membranes are flat disks that minimize the bending energy at the cost of the edge energy, and enclosed vesicles that minimize the edge energy at the cost of bending energy. In our work, the transition from disk to vesicle is studied theoretically using the string method, which is designed to find the minimum energy path (MEP) or the most probable transition path between two local minima of an energy landscape. Previous studies of disk-to-vesicle transition usually approximate the transitional states by a series of spherical cups, and found that the spherical cups do not correspond to stable or meta-stable states of the system. Our calculation demonstrates that the intermediate shapes along the MEP are very different from spherical cups. Furthermore, some of these transitional states can be meta-stable. The disk-to-vesicle transition pathways are governed by two scaled parameters, $\kappa G/k$ and $\gamma R_0/4k$, where $R_0$ is the radius of the disk. In particular, a meta-stable intermediate state is predicted, which may correspond to the open morphologies observed in experiments and simulations.

1:15PM J39.00011 Hybrid Lipid as Biological Surfactant, Robert Brewster, Weizmann Institute of Science, Phil Pincus, University of California- Santa Barbara, Sam Safran, Weizmann Institute of Science — Systems capable of forming finite-sized, equilibrium domains are of biological interest in the context of membrane rafts where it has been observed that certain cellular functions are mediated by small (nanometric to tens of nanometers) domains with specific lipid composition that differs from the average composition of the membrane. These small domains are composed mainly of lipids with completely saturated hydrocarbon tails that show good orientational order in the membrane. The surrounding phase consists mostly of lipids with at least one unsaturated bond in the hydrocarbon tails which forces a “kink” in the chain and inhibits ordering. In vitro, this phase separation can be replicated; however, the finite domains coarsen into macroscopic domains with time. We have extended a model for the interactions of lipids in the membrane, akin to that developed in the group of Schick (Elliott et al., PRL 2006 and Garbes Putzel and Schick, Biophys. J. 2007), which depends entirely on the local ordering of hydrocarbon tails. We generalize this model to an additional species and identify a biologically relevant component, a lipid with one fully saturated hydrocarbon chain and one chain with at least one unsaturated bond, that may serve as a line-active component, capable of reducing the line tension between domains to zero, thus stabilizing finite sized domains in equilibrium.

1:27PM J39.00012 Distribution of Drug Molecules in Lipid Membranes: Neutron Diffraction and MD Simulations, Mohan Boggara, University of Houston, Ella Mihailescu, University of California, Irvine, Ramanan Krishnamoorti, University of Houston — Non-steroidal anti-inflammatory drugs (NSAIDs) e.g. Aspirin and Ibuprofen, with chronic usage cause gastro intestinal (GI) toxicity. It has been shown experimentally that NSAIDs pre-associated with phospholipids reduce the GI toxicity and also increase the therapeutic activity of these drugs compared to the unmodified ones. In this study, using neutron diffraction, the DOPC lipid bilayer structure (with and without drug) as well as the distribution of a model NSAID (Ibuprofen) as a function of its position along the membrane normal was obtained at sub-nanometer resolution. It was found that the bilayer thickness reduces as the drug is added. Further, the results are successfully compared with atomistic Molecular Dynamics simulations. Based on this successful comparison and motivated by atomic details from MD, quasi-molecular modeling of the lipid membrane is being carried out and will be presented. The above study is expected to provide an effective methodology to design drug delivery nanoparticles based on a variety of soft condensed matter such as lipids or polymers.

1:39PM J39.00013 Calcium-induced domain formation in mixed lipid monolayers, Wouter G. Ellenbroek, Department of Physics and Astronomy, University of Pennsylvania, David A. Christian, Chemical & Biomolecular Engineering and the Laboratory for Research on the Structure of Matter, University of Pennsylvania, Ilya Levtental, Institute for Medicine and Engineering, University of Pennsylvania, Andrea J. Liu, Department of Physics and Astronomy, University of Pennsylvania, Paul A. Janney, Departments of Physics and Astronomy, and Bioengineering, University of Pennsylvania — Multivalent ions such as calcium play an important role in soft matter and biological systems. This role cannot be captured by a mean field treatment of the electrostatics such as the Poisson-Boltzmann equation, which neglects, for example, the fact that $Ca^{2+}$ ions can mediate attractions between negatively-charged objects. We show both experimentally and theoretically, that $Ca^{2+}$-mediated attractions lead to phase separation of charged and neutral lipid molecules in mixed lipid monolayers, and discuss the dependence on pH, salt concentration and ion valency.

1:51PM J39.00014 Membrane Disruption Mechanism of Antimicrobial Peptide, Kin Lok H. Lam, University of Chicago, Ting Ann Siah Team, Yuji Ishitsuka Team, Ka Yee C. Lee Team — PG-1, a cationic antimicrobial peptide, kills bacteria by forming pores which increase membrane permeability to ions or larger molecules. It has been proposed that PG-1 selectively induces stable membrane pores in bacterial membranes over mammalian membranes. To study the mechanism of action of PG-1, we directly visualize the topological changes induced by PG-1 in model membranes via atomic force microscopy for the first time. PG-1 induces structural transformations in supported lipid bilayers, progressing from bilayer edge instability, to the formation of pores, and finally to a network of wormlike micelles in a zwitterionic dimyristoylphosphatidylcholine model membrane with increasing PG-1 concentrations. The structural transformation can be understood in the framework of the action of 1d detergent, with PG-1 acting as a line active agent. The results elucidate the mechanism by which PG-1 uses to induce leakage in bacterial cells.

Tuesday, March 17, 2009 11:15AM - 2:15PM
Session J40 DBP: Biological Physics II 412
11:15AM J40.00001 Cell Rheology and Embryogenesis Using the Subcellular Element Model, Timothy Newman, Arizona State University — I will present recent work on grid-free computational modeling of both cell biomechanics and multicellular collective dynamics, the latter in the context of gastrulation in the chick embryo. Mechanics at both subcellular and multicellular scales is modeled seamlessly with the Subcellular Element Model (SEM). The SEM is able to capture basic viscoelastic properties of cells at a semi-quantitative level, and is efficient enough to simulate thousands of cells in three dimensions allowing computational analysis of biological hypotheses regarding collective cell motion during gastrulation. Work done in collaboration with Sebastian Sandersius, Arizona State University.

1 Funding provided by the Human Frontier Science Program.
11:51AM J40.00002 The effects of viscoelastic polymer substrates on adult stem cell differentiation. CHUNGHEUE CHANG, ADAM FIELDS, ALEX RAMEK, VLADIMIR JURUKOVSKI, MARCIA SIMON, MIRIAM RAFAILOVICH — Dental Pulp Stem Cells (DPSCs) are known to differentiate in either bone, dentine, or nerve tissue by different environment signals. In this study, we have determined whether differentiation could only through modification of the substrate mechanics. Atomic Force Microscopy (AFM) on Shear Modulation Force Microscopy (SMFM) mode indicated that the spun-cast polybutadiene (PB) thin films could be used to provide different stiffness substrates by changing the thicknesses of thin films. DPSCs were then plated on these substrates and cultured in standard media. After 28 days incubation, Laser Scanning Confocal Microscopy (LSCM) with mercury lamp indicated that the crystals were observed only on hard surfaces. The Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray analysis (EDX analysis) indicated that the crystals are calcium phosphates. The Glancing Incidence Diffraction (GID) was also used to determine the structure of crystals. These results indicate that DPSCs could be differentiated into osteoblasts by mechanical stimuli from substrate mechanics.

12:03PM J40.00003 Translocation of double strand DNA into a biological nanopore¹. SUNITA CHATKAEW, LAMIA MLAYEH, MARC LEONETTI, FABRICE HOMBLE, SFMB COLLABORATION — Translocation of double strand DNA across a unique mitochondrial biological nanopore (VDAC) is observed by an electron transport chain. Characteristics of opened and sub-conductance states of VDAC are studied. When the applied electric potential is beyond 20 mV, VDAC transits to a sub-conductance state. Plasmids (circular double strand DNA) with a diameter greater than that of the channel shows the current reduction into the channel during the interaction but the state with zero-current is not observed. On the contrary, the interaction of linear double strand DNA with the channel shows the current reduction along with the zero-current state. These show the passages of linear double strand DNA across the channel and the electrostatic effect due to the surface charges of double strand DNA and channel for circular and linear double strand DNA.

¹FNRS, Ecole Centrale de Marseille

12:15PM J40.00004 On-chip growth of polymeric nanowires for electro-mechanical probing of live cells. BRET FLANDERS, PREM THAPA, Kansas State University — This study characterizes the directed electrochemical nanowire assembly of amorphous polythiophene nanowires on micro-electrode arrays. In this approach, a long range component of an applied voltage signal defines a channel of maximum flux in the laboratory reference frame. Amorphous wires lack a natural growth axis. However, because polymerization is restricted to the channel-region, such materials may be grown with wire-like geometries, and the growth path of these wires may be controlled. The wire-laden electrode arrays are useful substrates for cell physiological studies. To this end, non-invasive methodology for inducing single Dictyostelium cells to approach and attach individual pseudopods to the tips of the polymeric wires will be presented.

12:27PM J40.00005 What do cell rheology experiments really measure? JOHN C. CROCKER, Chemical and Biomolecular Engineering, University of Pennsylvania — It is now widely appreciated that normal tissue morphology and function rely upon cells' ability to sense and generate forces appropriate to their correct tissue context. While the effects of forces on cells have been studied for decades, our understanding of how those forces propagate through and act on different cell structures remains at an early stage. The last decade has seen a resurgence of interest, with a variety of different micromechanical methods in current use that probe cells dynamic deformation in response to a time varying force. Recently, it has been shown that the seemingly disparate findings from different labs can be fit into a single, workable consensus description. The ability of researchers to carefully measure the mechanical properties of cells subjected to a variety of pharmacological and genetic interventions, however, currently outstrips our ability to quantitatively interpret the data in many cases. Despite these challenges, the stage is now set for the development of detailed models for cell deformability, motility and mechano-sensing that are rooted at the molecular level.

1:03PM J40.00006 Cargo transport by several molecular motors. STEFAN KLUMPFF, Center for Theoretical Biological Physics, UC San Diego, MELANIE MÜLLER, JANINA BEEG, RUMIANA DIMOVA, REINHARD LIPOWSKY, MPI of Colloids and Interfaces, Potsdam, Germany — In cells, cargoes are often transported by small teams of molecular motors rather than by a single motor. Furthermore, many cargoes perform bidirectional movements, which are based on the presence of two motor species on the cargo. We study the transport by several motors theoretically using a model that describes the stochastic binding and unbinding of motors from filaments and that is based on the properties of individual motors as observed in single molecule experiments. We find that the cooperation of several motors leads to a strongly increased run length, which is confirmed experimentally for beads pulled by several kinesin motors. Furthermore, such cargoes exhibit a non-linear force-velocity relation. For the case of two motor teams pulling into opposite direction we find that a stochastic tug-of-war model, where the motors interact only by pulling their common cargo into opposite directions, leads to surprisingly complex motility. In particular, even for two motor teams with equal strength, we find that a tug-of-war leads to fast bidirectional motion similar to what is observed in cells and usually taken as evidence for some unknown coordination mechanism. This behavior is due to a dynamic instability, which arises from the strong force-dependence of the rate with which motors unbind from filaments.

1:15PM J40.00007 Adverse Effects of TiO₂ Nanoparticles on Human Dermal Fibroblasts and How to Protect Cells. ZHI PAN, WILSON LEE, LENNY SLUTSKY, Stony Brook University, SOWMYA SANDARESH, Hixville High School, NICOLE ELSTEIN, Bayport-Bluepoint High School, RICHARD CLARK, NADINE PERNODET, MIRIAM RAFAILOVICH, Stony Brook University — We have studied the effects of exposure of human dermal fibroblasts to rutile and anatase TiO₂ nanoparticles. We found that these particles can impair cell functions, with the latter being more potent at producing damage. We showed that the exposure to nanoparticles decreases cell area, cell proliferation, mobility, and ability to contract collagen. Individual particles are shown to penetrate easily through the cell membrane, in the absence of endocytosis, while some endocytosis is observed for larger particle clusters. Once inside, the particles are sequestered in vesicles, which continue to fill up with increasing incubation time till they rupture. We also tested particles that were coated with a dense grafted polymer brush and, using flow cytometry, showed that the coating prevented the particles from adhering to the cell membrane and hence penetrating the cell, which effectively decreases reactive oxygen species (ROS) formation and protects cells, even in the absence of light exposure. Considering the broad applications of these nanoparticles in personal health care products, the functionalized polymer coating can potentially play an important role in protecting cells and tissue from damage.

1:27PM J40.00008 Surface Morphological Studies on Nerve Cells by AFM. GOKSEL DURKAYA, Department of Physics & Astronomy, Georgia State University, LEI ZHONG, VINCENT REHDER, Department of Biology, Georgia State University, NIKOLAUSS DIETZ, Department of Physics & Astronomy, Georgia State University — Surface morphological properties of fixed and living nerve cells removed from the buccal ganglion of Helisoma trivolvis have been studied by using Atomic Force Microscopy (AFM). Identified, individual neurons were removed from the buccal ganglion of Helisoma trivolvis and plated into poly-L-lysine coated glass cover-slips. The growth of the nerve cells was stopped and fixed with 0.1% Glutaraldehyde and 4% Formaldehyde solution after extension of growth cones at the tip of the axons. Topography and softness of growth cone filopodia and overlying lamellipodium (veil) were probed by AFM. Information obtained from AFM’s amplitude and phase channels have been used for determination of softness of the region probed. The results of structural studies on the cells are linked to their mechanical properties and internal molecular density distribution.
The four systems and comparisons with available data will be presented and discussed. The charge and spin distributions over them, and the associated hyperfine interactions of the nuclei of the atoms. Results and trends of these properties over aims in mind, we have studied quantitatively at a first principles level the electronic structures of all four halogen five liganded heme compounds, the natures of this purpose an in depth understanding at the electronic level of the heme units, the protein chains, and the interactions between the two, is vital. With these sign problem remains significant. I will discuss the different attempts we have made to reduce it.

For the composite excitations when momentum, such excitations have non-zero spectral weight at two distinct energy scales separated by the on-site repulsion are gapped composite excitations generated by the dynamics of the charge of Illinois, Urbana, Illinois 61801 — We show exactly that the only charged excitations that exist in the strong-coupling limit of the half-filled Hubbard model of Illinois, Urbana, Ilinois 61801 — We show exactly that the only charged excitations that exist in the strong-coupling limit of the half-filled Hubbard model of particles. The universal character of this theory is analogous to the van der Waals model for a liquid-gas transition. This work is supported by NIH R01 GM073082.

The four systems and comparisons with available data will be presented and discussed. The charge and spin distributions over them, and the associated hyperfine interactions of the nuclei of the atoms. Results and trends of these properties over

1:39PM J40.00009 Study of Charge and Spin Distribution Properties in Five-Liganded Halogen-Heme Systems, ARCHANA DUBEY, UCF Orlando, MINAKHI PUJARI, K. RAMANI LATA, SUNY Albany, ALYSSA GARCIA, A.F. SCHULTE, UCF Orlando, S.R. BADU, R.H. PINK, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, T.P. DAS, SUNY Albany, UCF Orlando — The current emphasis in biological physics is on the study of the functions of important systems, like for instance hemoglobin and cytochromes at a quantitative level. For these studies an accurate knowledge of the electronic structures of the entire molecules as well as parts of them are very important. In the heme proteins there is great current interest in both electron transport and in attachment and detachment of O₂, CO, and NO molecules to the iron. For this purpose an in depth understanding at the electronic level of the heme units, the protein chains, and the interactions between the two, is vital. With these aims in mind, we have studied quantitatively at a first principles level the electronic structures of all four halogen five liganded heme compounds, the natures of the charge and spin distributions over them, and the associated hyperfine interactions of the nuclei of the atoms. Results and trends of these properties over the four systems and comparisons with available data will be presented and discussed.

1:51PM J40.00010 Kalman meets neuron - the intersection of control theory and neuroscience, STEVEN SCHIFF, Penn State University — Since the 1950s, we have developed mature theories of modern control theory and computational neuroscience with almost no interaction between these disciplines. With the advent of computationally efficient nonlinear Kalman filtering techniques, along with improved neuroscience models which provide increasingly accurate reconstruction of dynamics in a variety of important normal and disease states in the brain, the prospects for a synergistic interaction between these fields are now strong. I will show recent examples of the use of nonlinear control theory for the assimilation and control of single neuron dynamics, a novel framework for dynamic clamp, the modulation of oscillatory wave dynamics in brain cortex, a control framework for Parkinsonian dynamics and seizures, and the use of optimized parameter model networks to assimilate complex network data.

2:03PM J40.00011 Protein Thermodynamics from Maxwell Constraint Counting, DONALD JACOBS, Department of Physics and Optical Science, UNC-Charlotte, DENNIS LIVESAY, Department of Bioinformatics and Genomics, UNC-Charlotte, OLEG VOROV, Department of Physics and Optical Science, UNC-Charlotte — Topological properties of network rigidity explain essential aspects of structural phase transitions and thermodynamic stability in proteins [1]. We present an exact transfer matrix method within a Distance Constraint Model (DCM) that maps interactions into distance constraints having energy and entropy contributions. Conformational entropy is reduced by interactions that rigidify structure, associated with independent constraints. Here, we solve the DCM using a mean-field treatment that assumes distance constraints are well distributed throughout the structure, meaning a distance constraint is independent until the structure is globally rigid. Experimental heat capacity curves are described markedly well with a few adjustable parameters. The universal character of this theory is analogous to the van der Waals model for a liquid-gas transition. This work is supported by NIH R01 GM073082.

2:17AM J41.00001 Origin of the Mott Gap, PHILIP PHILLIPS, ROBERT G. LEIGH, Loomis Laboratory of Physics, University of Illinois, Urbana, Illinois 61801 — We show exactly that the only charged excitations that exist in the strong-coupling limit of the half-filled Hubbard model of Fermi gas at unitarity, obtained through DiagMC simulation.

2:27AM J41.00002 Diagrammatic Monte Carlo, KRIS VAN HOUCKE, FELIX WERNER, UMASS Amherst, EVGENY KOZIK, ETH Zurich, LODA POLLET, NIKOLAY PROKOF’EV, BORIS SVISTUNOV, UMASS Amherst, DARPA OLE COLLABORATION — Diagrammatic Monte Carlo (DiagMC) is an exact technique that allows one to simulate quantities specified in terms of diagrammatic expansions, the latter being a standard tool of many-body quantum statistics. The sign problem, that is typically fatal to Monte Carlo approaches, appears to be manageable with DiagMC. We introduce a general DiagMC scheme for strongly interacting fermions. As an illustrative example, we discuss the application of DiagMC to the Fermi-Hubbard model, and benchmark the technique against state-of-the-art numerical tools for strongly correlated fermions. In addition, we discuss the thermodynamic properties of a Fermi gas at unitarity, obtained through DiagMC simulation.

2:39AM J41.00003 Unconventional soft gaps in strongly-correlated systems with coexisting short-range interaction and disorder, HIROSHI SHINAOKA, MASATOSHI IMADA, Dept. of Applied Physics, Univ. Tokyo — We report a theoretical study of the Anderson-Hubbard model under coexisting short-range interaction and disorder, which is one of the minimum models of real strongly-correlated materials. We determined the ground-state phase diagram in three dimensions within the unrestricted Hartree-Fock approximation. Although only short-range interaction is present, we found a soft gap in the single-particle density of states of the insulating phases [1]. This unconventional soft gap (soft Hubbard gap) cannot be explained within the conventional theory [2] which ascribes the formation of soft gaps to the long-range part of the Coulomb interaction. We present a phenomenology to clarify the origin of the soft Hubbard gap. We propose a multi-valley energy landscape as their origin. Further support by the exact diagonalization in one dimension beyond the mean-field level is given. Possible experiments to verify the present theory are also proposed. [1] H. Shinaoka and M. Imada, arXiv:0811.2492v1. [2] A. L. Efros and B. I. Shklovskii, J. Phys. C 8, L49 (1975).

2:51AM J41.00004 Determinant Quantum Monte Carlo method applied to the t-J model, ALEKSANDER ZUJEV, UC Davis, RICHARD FYE, 825 La Charles NE Albuquerque, NM 87123, RICHARD SCALETTAR, UC Davis — The usual approach to simulating the t-J model with the Determinant Quantum Monte Carlo (DQMC) method starts with the Hubbard model with a finite on-site interaction $U$ which is then increased to “almost” infinity. This approach, however, has considerable difficulties with large round-off errors (stability) and variances, and also a very bad fermion sign problem. In this talk, we will describe a different approach which starts with (almost) infinite $U$ by means of a projector operator and further prohibiting double occupancy by using a modified creation operator. The new technique will be shown to solve some of these difficulties. Unfortunately, the sign problem remains significant. I will discuss the different attempts we have made to reduce it.
We consider a coupled non-interacting and spin-density-wave (SDW) chains as an example. We find that the interchain hopping induces a short-rang SDW order in the extended Anderson-Hubbard model. Since the phase transition is believed to be of Kosterlitz-Thouless type, no local order parameter can describe such a transition. We find instead that the nodal regions and a pseudogap in the antinodal regions at lower dopings \( x \) (induced by strong short ranged order) than as a Mott phenomenon. Doping the gapped phase leads to a non-Fermi-liquid state with a Fermi surface only in theory is used to investigate the metal-insulator transition in the Hubbard model. At half filling a gap-opening transition is found to occur as the interaction increases beyond a critical value. The gapped behavior found in the 4-site DCA approximation is shown to be associated with the onset of strong antiferromagnetic and singlet correlations and the transition is found to be potential energy driven. It is thus more accurately described as a Slater phenomenon (induced by strong short ranged order) than as a Mott phenomenon. Dopping the gapped phase leads to a non-Fermi-liquid state with a Fermi surface only in the nodal regions and a pseudogap in the antinodal regions at lower dopings \( x \leq 0.15 \) and to a Fermi liquid phase at higher dopings.

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References:

1:03PM J41.00010 Effect of nonlocal interactions on the disorder-induced zero-bias anomaly in the extended Anderson-Hubbard model1, RACHEL WORTIS, HONGYI CHEN, W.A. ATKINSON, Trent University — Adding disorder to a system of correlated electrons moves single-particle states away from the Fermi surface. In the weakly correlated regime, consensus exists on the evolution of the resulting density of states anomaly between the limits of weak and strong disorder. Recently a number of groups have made progress in understanding the strongly correlated regime, mostly in the context of purely local interactions. We study the extended Anderson-Hubbard model using exact diagonalization on two-dimensional 12-site clusters, exploring the evolution of the zero-bias anomaly with the strength of the nonlocal interaction and with doping. At half filling, an exchange-driven Altshuler-Aronov-like anomaly develops Efros-Shklovskii-like atomic character and moves to a regime of strong charge-density correlations, whereas at quarter filling both the Efros-Shklovskii-like behavior and the charge density correlations are much weaker.

1Financial support provided by NSERC of Canada and SHARCNET.

1:15PM J41.00011 Local Order and the gapped phase of the Hubbard model: a plaquette dynamical mean field investigation. EMANUEL GULL, PHILIPP WERNER, ETH Zurich, XIN WANG, Columbia University, MATTHIAS TROYER, ETH Zurich, ANDREW MILLIS, Columbia University — The four-site DCA method of including intersite correlations in the dynamical mean field theory is used to investigate the metal-insulator transition in the Hubbard model. At half filling a gap-opening transition is found to occur as the interaction increases beyond a critical value. The gapped behavior found in the 4-site DCA approximation is shown to be associated with the onset of strong antiferromagnetic and singlet correlations and the transition is found to be potential energy driven. It is thus more accurately described as a Slater phenomenon (induced by strong short ranged order) than as a Mott phenomenon. Dopping the gapped phase leads to a non-Fermi-liquid state with a Fermi surface only in the nodal regions and a pseudogap in the antinodal regions at lower dopings \( x \leq 0.15 \) and to a Fermi liquid phase at higher dopings.

12:03PM J41.00005 Ordering and Frustration in a Strongly Correlated Chain system. SIDDHARTHA LAL, Department of Physics, University of Illinois at Urbana-Champaign, MUKUL LAAD, Max Planck Institute for Complex Systems, Dresden, Germany — We present recent results of our study on the one-dimensional extended Hubbard model with longer-range Coulomb interactions at quarter-filling in the strong coupling limit. With the complex phase diagram of the TMTSF and TMTTF organic charge transfer salts as motivation, we explore the possible charge and spin ordered states that arise from frustrating interactions. We find a quantum critical point in the phase diagram of the single chain and present results for some response functions in the quantum critical regime. RPA studies of coupled chains reveal a phase diagram with the ordered phase extended to finite temperatures and a phase boundary again ending at a quantum critical point. Critical quantum fluctuations at the QCP enhance the transverse dispersion, leading to a dimensional crossover and a low temperature transition from insulating chains to anistropic metallic bulk behaviour. These results have been reported in arxiv:0708.2156 and are in press at Int. J. Mod. Phys. B.

12:15PM J41.00006 Mott and Wigner-Mott transition away from half-filling. CHUNHUA LI, ZIQIANG WANG, Boston College — We study the Mott transition in strongly correlated electron systems away from half-filling in the presence of finite-range Coulomb interaction and/or a superstructure associated with an inhomogeneous electronic state. Using a cluster Gutzwiller approach, we map a minimal single band \( t-t'V-\Delta \) model with nearest neighbor Coulomb repulsion \( V \) and superlattice potential \( \Delta \), to a two-orbital Hubbard model with intra and interorbital Coulomb repulsion \( U \) and \( U' \) and a crystal field splitting \( \Delta \). We obtain the Mott transition at quarter-filling from both uniform and \( \sqrt{x}+\sqrt{1-x} \) charge density wave metals and discuss the physics of the Mott and Wigner-Mott metal-insulator transition.

12:27PM J41.00007 Effect of Interchain Hopping on Nonequivalent Hubbard Chains. TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, Japan, HIROYUKI YOSHIZUMI, TAKAO MORINARI — Motivated by recent report on the presence of different orders in each CuO\(_2\) plane and their coexistence in multi-layered high-temperature superconductors, we examine a simple model with two nonequivalent Hubbard chains coupled by interchain hopping, employing the density-matrix renormalization group (DMRG) and a mean-field calculation. We consider a coupled non-interacting and spin-density-wave (SDW) chains as an example. We find that the interchain hopping induces a short-rang SDW order from adjacent SDW chain and the induced order decreases with increasing the original SDW order of the adjacent chain. We discuss the finding in connection with the multi-layered cuprates.

12:39PM J41.00008 High Precision QMC Study of the 2D Hubbard Model. CHRISTOPHER VARNEY, SIMONE CHIESA, RICHARD SCALETTAR, University of California, Davis — The Hubbard model has provided insight into a wide variety of strongly correlated systems, including the cuprates and manganites. Recent advances in the generation of optical lattices allow for the possibility of experimentally studying the 2D Hubbard model in a new context. To enhance our understanding of the model, we examine the magnetic correlations on a rectangular lattice using Determinant Quantum Monte Carlo. In this talk, we discuss high precision calculations of the anti-ferromagnetic order parameter as a function of interaction strength and the effect of the aspect ratio on finite size scaling.

12:51PM J41.00009 Quantum phase transition in the one-dimensional half-filled asymmetric Hubbard model. YANG LIU, WEN-LING CHAN, SHI-JIAN GU, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong — We study the quantum phase transition in the one-dimensional asymmetric Hubbard chain at half-filling in terms of spin stiffness by the exact diagonalization method. Since the phase transition is believed to be of Kosterlitz-Thouless type, no local order parameter can describe such a transition. We find instead that spin stiffness might be able to describe the quantum phase transition since the spin degree of freedom is gapless in the Hubbard region, while gapful in the Falicov-Kimball region.
1:30PM J41.00003 One-dimensional periodic Anderson model at partial band filling , MIKLÖS GULACSI, IAN MCCULLOCH, Max Planck Institute for the Physics of Complex Systems — An effective Hamiltonian is derived for the one-dimensional periodic Anderson model via bosonization. The effective Hamiltonian is shown to reproduce all the features of the model as identified by DMRG and provides new information on the ferromagnetic to paramagnetic phase transitions and the paramagnetic phase. We are using a non-Abelian DMRG to determine numerically the phase diagram of the one-dimensional periodic Anderson model. We found very good agreement between the bosonization approach and the DMRG results.

1:51PM J41.00014 The Marginal Fermi Liquid-A Derivation Based on Dirac’s Constraints , D. SCHMELTZER, CCNY — Dirac’s method for constraints is used for enforcing the exclusion of double occupancy for Correlated Electrons. The constraint is given by the pair $Q(\mathbf{x}) = \psi(\mathbf{x})\psi(\mathbf{x})$ which annihilates the ground state $|\Psi\rangle$. Away from half fillings $Q(\mathbf{x})$ is replaced by a set of first class constraints $Q_{\mu}^{\alpha}Q_{\mu}^{\beta}$ which are restricted to negative energies. The propagator for the single hole is determined by a measure which is a function of time duration for the hole propagator. a)-The imaginary part of the self energy - is linear in the frequency. b)-In the superconducting phase the tunneling density of states is asymmetric.

2:00PM - 2:00PM —
Session K1 Poster Session II (2-5:00pm): Education; SPS/Undergrad Research; Metals; Magnetism; Instrumentation and Measurements; Chemical Physics; Artificially Structured Materials; Surfaces, Interfaces and Thin Films; AMO Physics; Quantum Information; Bio Physics Exhibit A

K1.00001 PHYSICS EDUCATION —

K1.00002 Stokes analysis of an optical system , GEORGI GEORGIEV, Assumption College, THOMAS SLAVKOVSKY, Assumption College, ASSUMPTION COLLEGE TEAM — As a transfer from research to teaching we are using stokes analysis to represent changes in the vectors for polarization of light as acted upon by the matrices of optical elements in undergraduate physics lab. The goal is to integrate students’ knowledge for matrix analysis with an experimental determination of the changes in the polarization of light. This method allows students to learn how to design an optical system by using mathematical analysis, a skill necessary for future scientists or engineers in the fields of optics. We have tested and implemented the lab. The results are that it is well accepted by the students, but is very involved computationally, and needs to be shortened. The Stokes analysis needs to be introduced earlier in the curriculum in order to make the students comfortable with the formalism.

K1.00003 The Doppler Effect in Sound Waves, Light Waves, and Quantum Waves , ALAN M. KADIN, Princeton Junction, NJ — In undergraduate modern physics courses, special relativity and quantum mechanics are generally introduced as a series of sharp breaks from classical physics. An alternative approach is suggested, focusing on the Doppler effect, closely related to changes in reference frames. In the classical acoustic Doppler effect with a source or observer moving with speed $u$, the frequency $f$ shifts while the wavelength $\lambda$ must remain fixed for classical transformations. Hence the phase velocity $v_{ph}=f\lambda$ must also shift. In the optical Doppler effect, $f$ also shifts for $u$ approaching $c$, but this must be accompanied by a corresponding shift in $\lambda$ (from the Lorentz transformation) in order to maintain $v_{ph}=c$ constant. The Doppler effect is usually not considered for quantum waves, but this clearly requires a non-classical shift in the de Broglie wavelength $\lambda=h/mv$ even for $u<c$. This shift is fully explained by the Lorentz transformation if one takes $f=mc^2/h$, as was shown by de Broglie in his original 1924 paper. This is a dispersive wave with $v_{ph}=c^2/v$, but a group velocity $v_g=v$, as required for a consistent physical interpretation. This emphasizes the relativistic basis of quantum waves.

K1.00004 Kinematic analysis of the Cretaceous Era dinosaur footprints near the Paluxy River, Texas: Predation event or not? , SCOTT LEE, University of Toledo — Motivation is enhanced by challenging students with interesting and open-ended questions. In this talk, a methodology for studying the locomotion of extinct animals based on their footprint tracks is developed and applied to a possible predation event recorded in Cretaceous Era deposits Students usually love learning about dinosaurs, an unexpected treat in a physics class. This example can be used in the classroom to help build critical thinking skills as the students decide whether the evidence supports a predation scenario or not.

K1.00005 Locomotion speeds of various dinosaurs , MARY DOUGHERTY, SCOTT LEE, University of Toledo — Most students have a passing curiosity about dinosaurs. Piquing this interest is an excellent tool to engage students. A methodology for estimating the locomotion speed of an animal based upon their footprint tracks is developed. Using this technique, an analysis of the locomotion speeds of various dinosaurs is performed. The tracks studied include 28 theropods (meat-eating dinosaurs), 23 sauropods (the “long-necked” herbivores), 28 non-armored, non-sauropod herbivores and 10 armored, non-sauropod herbivores. The theropods show the fastest locomotion speed as well as the greatest variety of speeds while the armored dinosaurs are the slowest.

K1.00006 Avogadro: Free, Open Source, Cross-Platform Computer Program for Building Molecules and Visualizing Structure , MARCUS HANWELL, GEOFFREY HUTCHISON, University of Pittsburgh — The Avogadro project is a free, open source approach to building chemical structures. It has integrated analysis, and three-dimensional visualization capabilities. Avogadro also uses external packages to perform quantum structure calculations. The work presented here illustrates a novel approach to working with the results of quantum calculations by visualizing possible molecular orbitals and allowing the user to select orbitals of interest. The Avogadro program allows the user to prepare new jobs for various quantum codes such as GAMESS-US, Q-Chem, Gaussian and Molpro. Due to the plugin-based nature of the Avogadro project many specialized options can be added, such as raytracing the electronic structure of the molecule to produce high quality output, building carbon nanotube structures, or designing solid-state structures. Avogadro is already being used by educators and researchers. Due to the free and open source nature of the project, it can be readily downloaded and used by all students in and out of the classroom. It can also be tailored to particular institutions and/or courses.
K1.00007 Gaps and Tails: The restricted N-body problem in colliding galaxies and the asteroid belt . ANNA PANCOAST, SHEA GARRISON-KIMMEL, PETER LOVE, Haverford College — We report simulations of the restricted n-body problem performed in the class Computational Physics at Haverford College. We simulated gravitational interactions in a large system in which nearly all of the particles, such as asteroids or stars, are assumed to have no effect on the trajectories of other particles. We begin by simulating the emergence of Kirkwood Gaps in the asteroid belt. We then modify the code to include the extensive initial conditions necessary to model the parabolic collision of two galaxies. We explored both direct and retrograde passages between the galaxies, reproducing the results of the 1972 paper by Toomre and Toomre, specifically the formation of galactic bridges and tails.

K1.00008 Understanding Statistical Mechanics and Biophysics Using Excel , PETER NELSON, Benedictine University — A new approach to teaching statistical mechanics and biophysics is presented using the classic two-box system from statistical mechanics as an example. This approach makes advanced physics concepts accessible to a broad audience including undergraduates with no calculus background. Students develop a simple Excel spreadsheet that implements a kinetic Monte Carlo (kMC) simulation algorithm “from scratch”. The students discover for themselves the properties of the system by analyzing the simulation output in a directed, activity-based exercise. By changing the number and initial distribution of the particles, students see how the system approaches equilibrium and how system variability changes with system size. A finite difference solution is also implemented in Excel, and students compare its predictions with the kMC results. This approach is quite different from using “canned” computer demonstrations, as students design, implement and debug the simulation themselves – ensuring that they understand the model system intimately.

K1.00009 Computational Physics Undergraduate Research Experience (A case Study) , HOMEYRA SADAGHIANI, ALEX SAML, California Polytechnic University Pomona — There is a growing trend of inclusion of more research programs into undergraduate education. In spite of that, the assessment of undergraduate-research experience in physics is limited. This presentation describes a ten weeks undergraduate summer research experience in computational physics in the field of biophysics for two upper division physics students at Cal Poly Pomona. The analysis of Pre/post test data suggests more gains on research methodologies and skills than actual physical concepts underlying the research project. We also discuss student attitude change measured by survey and interviews.

K1.00010 Scientific Inquiry: A Problem-Based Approach for Improving Teaching and Learning , PETER SHELTON, PEGGY SCHIMMOELLER, TATIANA TOTEVA, Randolph College — We describe a research project that had two goals: (1) to design and develop a content specific science inquiry institute to improve teachers’ instructional practices in the sciences and thus students’ achievement in science; and (2) to investigate students’ perception of scientists as a measure of their attitude toward science, and to see whether an inquiry science curriculum can improve attitudes. We report that certain stereotypical images of scientists are prevalent among students. Teacher participants increased content knowledge and familiarity with using inquiry and hands-on methods in the classroom.

K1.00011 To Click or Not to Click1 , NINA ABRAMZON, HOMEYRA SADAGHIANI, California Polytechnic University Pomona — A comparison of clickers v. flashcards in a controlled setting was done to test a) whether clickers show an improvement over flashcards in students learning the following concepts: i) Coulomb’s force law and ii) magnetic fields caused by currents, and b) if students using clickers are more open towards conceptual questions and the peer instruction method compared to students using flashcards. Two classes taught concurrently by the same instructor were taught identically, except that in one class parach-goldenrod paradigm was used to ask conceptual questions using clickers, and in the other using flashcards. To test which students learned the concepts better, a few multiple choice questions from a standard exam used in physics education were included in the final exam of both classes, and the performance of the two classes was compared. In addition, a questionnaire was given to each class to evaluate students’ opinions about the benefits of lectures including conceptual TPS questions and the use of related conceptual questions on exams. The results of the survey were compared between the two classes. The experimental design and results of the study will be presented.

1Sponsored by the Faculty Center for Professional Development at Cal Poly Pomona.

K1.00012 SOCIETY OF PHYSICS STUDENTS AND UNDERGRADUATE RESEARCH –

K1.00013 Flexible Solution-Processed TiO2-Based Memory1 , BARBARA DUNLAP, NADINE GERGEL-HACKETT, BEHRANG HAMADANI, JOHN SUEHLE, CHRISTINA HACKER, DAVID GUNDLACH, CURT RICHTER — We have fabricated flexible titanium dioxide memory devices using a room temperature spin-on titanium dioxide (TiO2) sol gel technique. These devices show a non-volatile memory behavior with on/off ratios up to 10,000:1 and can be switched between low and high current states by applying an adequate bias (less than 10 V). Once switched, the state can be read by applying a small bias (0.5 V). The device can then be set back to the previous current state by applying a bias that is equal in magnitude but opposite in polarity to the initial bias. Devices maintain on/off ratios greater than four orders of magnitude when flexed 4,000 times, still switch after being flexed 8,000 times, and hold their set state for longer than 1x10^6 seconds. The advantages of our devices include that they are low power, rewritable, nonvolatile, lightweight, physically flexible, and they have a simple, inexpensive, two-terminal, room temperature processed device design.

1Work was done at the National Institute of Standards and Technology. Barbara Dunlap was a summer intern working at NIST through an internship with the Society of Physics Students.

K1.00014 Hydrogen storage media through nanostructured polymeric materials1 , SCOTT KIRKLIN, BRIAN DORNEY, SHENGWEN YUAN, PETER ZAPOL, Argonne National Laboratory, LUPINC YU, University of Chicago, Di-JIA LIU, Argonne National Laboratory, ARGONNE NATIONAL LABORATORY COLLABORATION, UNIVERSITY OF CHICAGO COLLABORATION — On-board hydrogen storage is critical to future transportation technologies such as H2-powered fuel cell vehicles. Reported here is our current effort in developing nanostructured polymeric materials as the non-dissociative hydrogen adsorbents for the transportation application. Various porous polymers were prepared. The discussion will be focused on the surface structural characterization using BET approach and hydrogen adsorption capacities and physical properties using a Sieverts type isotherm measurement. Details on improving the accuracy of measurement as well as data analysis will also be reported.

1This project is funded by the Department of Energy, Office of Energy Efficiency and Renewable Energy
A few percent. The results are relevant to recent experiments on the wetting of cesium by helium/hydrogen solutions, and may also have astrophysical applications. The results are relevant to recent experiments on the wetting of cesium by helium/hydrogen solutions, and may also have astrophysical applications.

We have been a number of reports on CNT based membrane electrode assembly (MEA) in PEMFC, but CNTs in these electrodes are oriented randomly and the advantages associated with the structural properties of CNTs were not fully utilized. We report here our progress in fabricating and evaluating MEAs made of catalyst decorated, vertically aligned carbon nanotube (ACNT) layers. For comparison, a commercial MEA prepared through the ink-based process was also tested under similar conditions. Improved performance was observed for ACNT-based MEAs, particularly at high current densities, suggesting enhancement in mass transport and improved water management.

This work was supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy.

K1.000080 K1.00015 Polymer Electrolyte Membrane Fuel Cell with Vertically Aligned Carbon Nanotube Electrode, ANN CALL, GABRIEL GOENAGA, JUNBING YANG, DI-JIA LIU, Argonne National Laboratory — Carbon nanotubes (CNTs) have been considered a promising material for various applications. Electro-catalyst support for polymer electrolyte membrane fuel cells (PEMFCs) is one of them. There have been a number of reports on CNT based membrane electrode assembly (MEA) in PEMFC, but CNTs in these electrodes are oriented randomly and the advantages associated with the structural properties of CNTs were not fully utilized. We report here our progress in fabricating and evaluating MEAs made of catalyst decorated, vertically aligned carbon nanotube (ACNT) layers. For comparison, a commercial MEA prepared through the ink-based process was also tested under similar conditions. Improved performance was observed for ACNT-based MEAs, particularly at high current densities, suggesting enhancement in mass transport and improved water management.

K1.000080 K1.00016 Measuring and Using the dn/dc of HPC Polymer and Microgel Solutions, KRISTA FREEMAN, KIRIL STRELETZKY, Cleveland State University — The specific refractive index increment (dn/dc), the change in index of refraction with concentration, is essential for accurate light scattering (SLS) experiments on polymer solutions. With a reliable value for dn/dc, SLS yields basic polymer properties such as radius of gyration, molecular weight, and second virial coefficient. This study focuses on determining dn/dc values of hydroxypropylcellulose (HPC) polymer and microgel solutions and practically applying these values in SLS. Using a differential refractometer, HPC solutions were analyzed at a range of concentrations, molecular weights, wavelengths, temperatures, and filtration protocols. It was determined that dn/dc of HPC polymer is independent of temperature in good solvents, slightly dependent on molecular weight, inversely proportional to wavelength squared, and sensitive to polymer solution’s filtration protocol. HPC microgel testing produced dn/dc values one order of magnitude larger than those of HPC polymer solutions and did not support the expected wavelength dependence. These findings were analyzed and used to obtain a molecular weight, radius of gyration, and second virial coefficient for HPC polymer and microgel solutions.

K1.000080 K1.00017 Measuring Insulation in Walls Using a Thermocouple to Measure Temperature Differences, BETH PARKS, CLAYTON BROWN, Colgate University — It would be useful to develop tools to measure building insulation non-invasively and inexpensively. The temperature difference across an exterior wall and the center of the room is a sensitive measure of the amount of insulation in the wall. We describe measurements using a thermocouple to determine the insulation in a mock house.

K1.000080 K1.00018 Lasing in Superconducting Qubits, ALYSSA WILSON, ROBERTO RAMOS, Drexel University — Qubits are superconducting circuits that have many interesting quantum properties similar to those displayed by atoms. One such behavior is lasing, as manifested in a resonator coupled to a qubit. I will review experiments in which lasing was exhibited in charge qubits and three-Josephson-junction flux qubits. I will also examine the similarities between these systems and compare these to properties of the Josephson phase qubit. In the presentation, I will discuss the feasibility of demonstrating this phenomenon in the phase qubit.

K1.000080 K1.00019 Evaluation and Redesign of Introductory Undergraduate Physics Series for Use with USB Devices, LEAH PARSONS, GARY BEDROSIAN, Allegheny College — The introductory physics laboratory series at many colleges suffers from several problems, including a large time commitment, inflexibility of lab set-ups, and lack of accommodation of multiple learning styles. It is difficult in a conventional lab set-up, in which students follow a carefully specified series of steps, to be able to generalize findings to more than one specific case. In this paper, we propose changes that will allow students to form the labs to their own learning styles better than the traditional approach. The integration of USB devices will allow this. We have reduced the current introductory physics labs at Allegheny College to their basic principles in order to apply them to a new, more flexible, lab paradigm. Using a USB device designed by Rensselaer Polytechnic Institute, labs that reflect the core concepts of introductory physics will be able to be performed in a more agreeable environment: the student’s own home, at a time of their choice, with use of a personal computer and simple additional materials. This project will present the method of lab design as well as proposed testing of lab effectiveness.

K1.000080 K1.00020 Measuring Proper Motion of Barnard’s Star, KATRINA WIECHMANN, TOM MICHALIK, Randolph College — Stars of the night sky are generally considered to be fixed points, not changing noticeably over generations of observations. While most stars seem to appear in the same place year after year, some change location noticeably, the best example being Barnard’s Star. Barnard’s star is closer to Earth than any other star except Proxima Centauri. It also appears to move across the sky faster than any other star. This change in apparent location is caused by the movements of our Solar System and the motion of the star in question, and is known as proper motion. Using the astrometric capabilities of the MIRA software along with precise positional information for reference stars from the Tycho satellite star catalogue, the position of Barnard’s star is computed relative to the reference stars. We calibrate a series of images of Barnard’s Star taken in the Randolph College Observatory between 2001 and 2008 in order to independently determine the proper motion of Barnard’s star and compare this measurement to the accepted value of \( 10.25 \)" per year.

K1.000080 K1.00021 Sync-map Description of Coupled Oscillators, GILAD BARLEV, Kenyon College, EDWARD OTT, MICHELLE GIVAN, University of Maryland, College Park — The Kuramoto model describes the tendency of coupled oscillators to synchronize when the coupling strength is above a critical value. Through Monte Carlo simulations, we study the behavior of a variation on the discrete-time Kuramoto model and verify certain properties of the model, namely the critical coupling value and the rate of relaxation towards synchronization. We then apply the model to non-directed networks with community structure to investigate synchronization within communities. Further, we propose a method for the discovery of community structure within networks based on observations of the time-averaged degree of synchronism between pairs of oscillators within our system.

K1.000080 K1.00022 Partial Molar Volume of Helium Dissolved in Hydrogen, MADELINE SMITH, M.S. PETTERSEN, Washington and Jefferson College — We have determined the partial molar volume \( v' \) of helium dissolved in hydrogen, by analyzing existing data on the concentrations of the liquid and the coexisting vapor phase at high pressures. The partial molar volume can be found from the chemical potential of the helium in solution \( (\mu_2 = \mu_{2s} + \mu_{2g}) \), where \( \mu_2 \) is the chemical potential of the helium in solution, and \( \mu_{2g} \) its concentration, and the chemical potential can be determined from pressure and the concentration of the vapor phase, after applying virial corrections. Both \( v' \) and the virial terms lead to corrections to Henry’s law. Over the range studied (0-50 bar and 15.5-29 K), we find that the partial molar volume of helium is equal to the molar volume of pure hydrogen, within a few percent. The results are relevant to recent experiments on the wetting of cesium by helium/hydrogen solutions, and may also have astrophysical applications.
K1.00023 Harmonic and Intermodulation Distortion in a Superconducting Microwave Resonator

K1.00024 The Depletion Layer: A mystery of Science

K1.00025 The Design and Construction of a Surface Plasmon Resonance Imaging Apparatus for the Study of Patched Hydrophobic and Hydrophilic Surfaces in Water

K1.00026 Computational Electromagnetics Post Processing Using 'MD-Grape' Board

K1.00027 Computational Electromagnetics: Adaptation of the MD_GRAPE Accelerator Board

K1.00028 Impact of barrier height distribution on tunneling conductance and extracted barrier parameters

K1.00029 ABSTRACT WITHDRAWN

K1.00030 Experimental study of plasma sheath conformation to rectangular depression

K1.00031 Synthesis of Nanosized Silicon Powders and Characterization of Their Electrical Properties
K1.00032 Electron Paramagnetic Resonance Spectroscopic Studies of Cyanide-Bridged Fe/Os and Fe/Ru Clusters, KATLYN MEIER, TANYA NOCERA, R. ABOOD, Allegheny College, Dept. of Physics, M. CHEN, Carnegie Mellon University, Dept. of Chemistry, M. HILFIGER, Texas A&M University, Dept. of Chemistry, D. PETASIS, Allegheny College, Dept. of Physics, C. ACHIM, Carnegie Mellon University, Dept. of Chemistry, K. DUNBAR, Texas A&M University, Dept. of Chemistry — The pertunecular, cyanide-bridged metal clusters with the general formula \([M(tmphen)2][M'(CN)6]2\) \((tmphen = 3, 4, 7, 8\text{-tetrathemethyl-1, 10-phenanthroline})\) have a core with trigonal bipyramidal geometry with equatorial \([M(tmphen)2](CN)2]\) and axial \([M'(CN)6]\) ions and contain M-CN-M' or M-NC-M' units, depending on the relative preference of the M and M' ions for the C or N terminus of the cyanide bridge. Spin-crossover behavior has been observed in these clusters and has motivated the current study. A series of Electron Paramagnetic Resonance (EPR) spectra of solid samples of the complexes with M/M' = Fe/Os and Fe/Ru were obtained between the temperatures of 2K and 300K. EPR spectra were also collected for samples dissolved in MeCN and MeOH. The EPR signals observed from Os (III) ions in the Fe/Os cluster and the signals from the Fe/Ru cluster indicating changes in oxidation and spin states of the metal ions as a function of temperature will be presented.

K1.00033 METALS —

K1.00034 Low energy positron sticking on surfaces — comparison of experiment and calculations, S. MUKHERJEE, K. SHASTRY, U. Texas at Arlington, N. G. FAZLEEV, U. T. Arlington, A. H. WEISS, U. Texas at Arlington — Recent measurements have provided evidence that low energy positrons incident upon a metal surface can make a single step transition from an unbound scattering state to an image potential bound state resulting in the creation of an electron-hole pair. Because the transition into the surface state results in the release of an additional \(\sim 3\) eV of energy as compared to a transition into a bulk state, the direct transition from scattering state to surface state can result in the creation of secondary electrons even at beam kinetic energies below the energy threshold necessary to generate secondary electrons in scattering processes in which the positron final state is a bulk state. In this poster we present a comparison of the experimental results with model calculations from which the rate of the direct process is estimated and the implications of these measurements in the understanding of quantum-sticking of positrons to surfaces are considered.

K1.00035 The Surface Dynamics of the Initial Oxidation Behavior of CuNi Alloys, STEVE ZIEMACK, LI SUN, JUDITH YANG, JEFF EASTMAN, GUANGWEN ZHOU, UNIVERSITY OF PITTSBURGH COLLABORATION, ARGON NATIONAL LABORATORY COLLABORATION, EUGENE, WASHINGTON — As an extension of our previous work on the initial oxidation stages of pure Cu and CuAu alloy, we are currently visualizing the oxidation of CuNi alloys by in-situ ultra high vacuum transmission electron microscope (UHV-TEM) and X-ray diffraction. We investigated systematically a range of CuNi (001) compositions, including 2.8,15 and 24 at\%Ni at P (O2) =5x10-4 torr and T=500-700°C. The initial oxidation behavior is similar to that of Cu (001) AND CuAu (001), where oxide islands rapidly nucleate, grow and coalesce. However, remarkable differences exist: 1) a second rapid nucleation of compact and dense oxide islands occurred and 2) polycrystalline oxides formed, where only cube-on-cube epitaxial Cu2O islands nucleated on Cu (001) and CuAu (001) for all temperature and pressures studied. The surface segregation behavior of Cu and Ni may explain these surprising results.

K1.00036 Creation and Characterization of Gold Coated Slides with a Home Built Deposition Chamber, NATE RIEDERS, ADELE POYNOT, Allegheny College — I discuss the creation of gold slides as part of a physics senior thesis at Allegheny College. The device used for making the gold slides was constructed as part of this project. Gold wire was placed in an evacuated chamber along with an array of glass slides. The gold wire is heated and evaporated onto the glass slides, leaving a thin deposition layer. The gold slides are created for the study of hydrophobic materials using surface plasmon resonance (SPR). The use of SPR as the experimental method requires the thickness of the gold layer to be precisely determined. Thus, the thickness of the gold slides is characterized using scanning tunneling microscopy.

K1.00037 Surface Layer Availability Approach to Systems with Solid-Fluid Surfaces, ROBERT CAMMARATA, Johns Hopkins University — Although the dividing surface method as devised by Gibbs can be used to completely describe the surfaces of fluid systems, in the case of fluid-solid interfaces with a finite size crystal the approach is generally restricted to systems where the solid is a single phase material. This is a result of the fact that the surface chemical potential of the solid component is not well-defined. As a result, Gibbs chose a dividing surface location where the surface excess amount of that component is zero so that the corresponding surface chemical potential was never needed. However this approach cannot be extended to systems containing multicomponent solids. It is proposed that for such systems a surface availability function, analogous to the thermodynamic availability function used in engineering thermodynamics, can be employed. It will be shown that such an approach can be used without the need of a particular dividing surface location, and that more generally the dividing surface construction can be dispensed with in favor of a finite volume surface layer. It is shown that by using this surface layer formulation a variety of problems, including surface adsorption and nucleation during solidification, can be rigorously treated for multicomponent systems.

K1.00038 Dielectric function trajectory of ultrathin gold films, XUEFENG WANG, DAVID NOLTE, Purdue University — There have been attempts to study the complex refractive index \(n_0\) of gold films by ellipsometry, but the measurements become unreliable when the average film thickness is below several nanometers, presumably because of optical anisotropy of the thin film. Here, we apply interferometric picoellometry to measure \(n_0\) by analyzing the Fourier-domain anisotropic diffraction of a normal-incidence scanning Gaussian laser beam reflected by a stripe-patterned gold film. The \(n_0\) and dielectric constant \(\varepsilon_g\) of the gold film were measured for thicknesses ranging continuously from 0.1 nm to 10 nm at a wavelength of 488 nm. Three distinct regimes of the \(\varepsilon_g\) trajectory on the complex plane were observed as the gold thickness increased. The first regime (gold thickness: 0.1 nm ~ 0.7 nm) reveals an evolution from sparse clusters to dense clusters. The real part of \(\varepsilon_g\) changes from 2.3 to 7.0 and the imaginary part changes from 0 to 0.7. The Maxwell-Garnett equation is applied for this regime by treating the film as an effective medium consisting of air and gold clusters. The second regime (0.7 nm~ 2 nm) is a linear curve of \(\varepsilon_g\) suggesting a transition from isolated clusters into a continuous thin film. The third regime (2 nm ~ 10 nm) shows a circular trajectory of \(\varepsilon_g\) moving towards the bulk value, which can be interpreted by the Drude equation.

K1.00039 The Variational Calculation for Small Cylindrical Metallic Cluster, CHIN-SHENG WU, Yuan Ze University — We use the Hohenberg-Kohn principle to calculate the density of the surface electronic charge around small cylindrical metallic cluster. The surface potential is varied in order to get the minimum total energy, which is the summation of electro-static energy and exchange-correlation energy. We use the availability function used in engineering thermodynamics, can be employed. It will be shown that such an approach can be used without the need of a particular dividing surface location, and that more generally the dividing surface construction can be dispensed with in favor of a finite volume surface layer. It is shown that by using this surface layer formulation a variety of problems, including surface adsorption and nucleation during solidification, can be rigorously treated for multicomponent systems.

K1.00039 The Variational Calculation for Small Cylindrical Metallic Cluster, CHIN-SHENG WU, Yuan Ze University — We use the Hohenberg-Kohn principle to calculate the density of the surface electronic charge around small cylindrical metallic cluster. The surface potential is varied in order to get the minimum total energy, which is the summation of electro-static energy and exchange-correlation energy. We use the local approximation for the inhomogeneous dielectric function around the surface. Therefore this surface charge can be applied to find dielectric constant, which is a function of the electron density. The dielectric constants are calculated on the cylindrical surface for various metal densities.
K1.00040 A Green Hydrothermal Synthesis for Iron-Doped, Carbon-Coated Tellurium Nanostructures and an Analysis of the Effects of the Molecular Weight and Ratio of Poly(vinylpyrrolidone) on Nanostructure Morphology¹, T. MULLIGER, Clemson University, S. MISHRA, The University of Memphis, S. GUHA, University of Missouri — A poly(vinylpyrrolidone) (PVP)-assisted hydrothermal process was used to synthesize tellurium nanostructures, as well as carbon-coated tellurium nanostructures (Te@C) in the presence of glucose as a carbon source. The thickness of ultra-thin tellurium nanostructures in the presence of PVP was found to depend upon the molecular weight of the polymer, as well as the ratio of polymer to tellurium source (Na2TeO3) used as starting materials. Structures ranging from 3-15nm were synthesized using four different molecular weights of PVP polymer (10,000; 29,000; 40,000; and 55,000) as well as different ratios of polymer to sodium tellurite, and their difference are compared. Varying the reaction time of the carbon-coating hydrothermal process yielded carbon-shell thickness ranging 20-60nm. As-prepared Te@C nanostructures were decorated with iron nanoparticles through an ultrasonication process at 70°C. Under a flow of Ar, hollow carbon nanostructures were also synthesized through a mild chemical treatment process at room temperature. Samples were extensively characterized using transmission electron microscopy (TEM), scanning electron microscopy and energy dispersive x-ray analysis (SEM/EDAX), ultraviolet visible, and PL.

¹Authors like to thank RC, PRF, and REU for the support of this project.

K1.00041 Polymer Assisted Core-shell Ag-C nanoparticles Synthesis via Green hydrothermal Technique, JAMES WILLIAMS, SANJAY MISHRA, The University of Memphis, Memphis, TN — Core-Shell Ag-C nanoparticles were synthesized in the presence of glucose through a one-pot green hydrothermal wet chemical process. An aqueous solution of glucose and Ag nitrate was hydrothermally treated to produce porous carbonaceous shell over silver core nanoparticles. The growth of carbon shells was regulated by either of the polymers (poly) vinyl pyrrolidone (PVP) or poly vinyl alcohol (PVA). The two polymers were compared to take a measure of different tunable sizes of cores, and shells. The effects of hydrothermal temperature, time, and concentration of reagents on the final formation of nanostructures were studied using UV-vis extinction spectra, transmission electron microscope, and Raman spectroscopy. The polymer molecules were found to be incorporated into carbonaceous shell. The resulting opacity of the shell was found to be hydrothermal time and temperature dependent. The shell structure was found to be more uniform with PVP than PVA. Furthermore, the polymer concentration was found to influence size and shape of the core-silver particles as well. The core-shellled nanoparticles have surfaces with organic groups capable of assembling with different reagents that could be useful in drug-delivery, optical nanodevices or biochemistry.

K1.00042 Growth Mechanism Study of Carbon Nanospheres Synthesized using Green Hydrothermal Technique, M. DOORLEY, Southwest Community College, Memphis, TN, S.R. MISHRA, M. MARADJI, S.K. KARNA, The University of Memphis, Memphis, TN, N. DUBENKO, N. ALI, Southern Illinois University, Carbondale, IL, E. GUNAPALA, K. MARASINGHE, University of North Dakota, Grandforks, ND — FeNi nanoparticles (NP) in the size range of 50 to 250 nm were synthesized via a wet chemical method. The precursor, sulfate salts of iron and nickel were reduced in alkaline media and in the presence of either polymers PEG (200-20,000 MW) or PVP (10,000 to 55,000 MW). The synthesis process was studied to understand the role of polymers in the growth of NP. TEM and XRD studies show formation of highly crystalline and well dispersed FeNi NP in polymer matrix. A decrease in particle size with an increase in PVP MW and increase in particle size with increase in PEG MW was observed. Furthermore, increase in PVP concentration leads to increase in particle size while increase in PEG concentration did not affect the particle size. Low temperature ZFC magnetization study show decrease in saturation magnetization value with the increase in polymer MW. It is concluded that the polymer mediated growth of FeNi NP involved 1) the formation of coordinative bonds between polymer and metal ions, 2) polymer-promoted nucleation, which produce small FeNi nanoparticles, and 3) steric shielding of the FeNi nanoparticles surfaces through chemical bonding to polymer which inhibited particle-particle contact and, thus the agglomeration of NP.

K1.00043 Polymer assisted synthesis of FeNi nanoparticles, S.K. KARNA, S.R. MISHRA, The University of Memphis, Memphis, TN, I. DUBENKO, N. ALI, Southern Illinois University, Carbondale, IL, E. GUNAPALA, K. MARASINGHE, University of North Dakota, Grandforks, ND — FeNi nanoparticles (NP) in the size range of 50 to 250 nm were synthesized via a wet chemical method. The precursor, sulfate salts of iron and nickel were reduced in alkaline media and in the presence of either polymers PEG (200-20,000 MW) or PVP (10,000 to 55,000 MW). The synthesis process was studied to understand the role of polymers in the growth of NP. TEM and XRD studies show formation of highly crystalline and well dispersed FeNi NP in polymer matrix. A decrease in particle size with an increase in PVP MW and increase in particle size with increase in PEG MW was observed. Furthermore, increase in PVP concentration leads to increase in particle size while increase in PEG concentration did not affect the particle size. Low temperature ZFC magnetization study show decrease in saturation magnetization value with the increase in polymer MW. It is concluded that the polymer mediated growth of FeNi NP involved 1) the formation of coordinative bonds between polymer and metal ions, 2) polymer-promoted nucleation, which produce small FeNi nanoparticles, and 3) steric shielding of the FeNi nanoparticles surfaces through chemical bonding to polymer which inhibited particle-particle contact and, thus the agglomeration of NP.

K1.00044 Adiabatic Electron-Phonon Coupling in the A15 Compounds V3Si, V3Ge and V3Co, OLIVIER DELAIRE, M. LUCAS, ORNL, M. KRESCH, B. FULTZ, Caltech — The phonon density of states (DOS) of the A15 compounds V3Si, V3Ge, and V3Co was measured as a function of temperature between 10K and 1273K with inelastic neutron scattering. The temperature dependence of the phonon DOS strongly departs from the predictions of the quasiharmonic model in the superconducting compounds V3Si and V3Ge, but behaves more normally in the non-superconducting V3Co. Using first-principles electronic structure calculations, the observed anomalies are related to the details of the band structure in these compounds. It is shown that sharp features in proximity to the Fermi level lead to anomalous phonons through a sensitivity to thermal disorder, or adiabatic electron-phonon coupling. In the case of V3Co, the sharp peak in the electronic DOS leads to a stiffening of the phonons with increasing temperature. It is shown that V3Si and V3Ge, a sharp peak in the electronic DOS leads to a stiffening of the phonons with increasing temperature. These results are compared to recent measurements of the phonon DOS and its temperature dependence in the B20 compounds Fe(1-x)Co(x)-Si.

K1.00045 Impurity Studies in CeCoIn5, ABBEKE KEBEDE, NC A&T State University, TERELL DIAL, NC A&T State University, NHHPL-LOS ALAMOS COLLABORATION — Systematic alloy studies of CeTIn5 (T = Co, Rh, Ir) reveal the stability of superconductivity in a wide range of composition; and in some cases it coexists with a magnetically ordered phase. We extended these studies to include (R, Ce)(Co,M)n; are (R= Pr and M= Fe, Mn). Our preliminary measurements indicate that the samples are single phase, and they exhibiting a wide range of transport and magnetic properties. In this communication we present the results of our resistivity and magnetic susceptibility measurements.

K1.00046 The 0.7 anomalous conductance¹, D. SCHMELTZER, Ccny-Cuny, A. KUKLOV, Csi-Cuny — At low electronic densities and finite temperatures the method of one dimensional Bosonization is not applicable. We introduce the zero modes method to incorporate Fermi Dirac Statistics. We compute the conductance at finite temperatures in the presence of long range Coulomb and biased umklapp interactions. We show that the 0.7 conductance anomaly appears at low densities when the Fermi energy and the temperature are of the same order of magnitude.

¹Ccny Collaborative grant -2007-2008
K1.00047 Quantum critical fluctuations in the itinerant antiferromagnet Nd$_2$O$_2$$_{29}$. JINGUANG CHENG, JIANSHI ZHOU, JOHN GOODENOUGH. TMI. University of Texas at Austin, HAIDONG ZHOU, NMHFL, Florida State University — Monoclinic Nd$_2$O$_2$$_{29}$ is a metallic antiferromagnet with $T_N \approx 12$ K. [1] We have studied critical behaviors near $T_N$ by measuring the resistivity ($\rho$), specific heat ($C_p$), and thermoelectric power ($S$). As $T_N$ is approached from $T_N^-$, critical behaviors used in ferromagnetic metals, $\rho/dT = (\alpha/\alpha)(T)-\beta + c^1 T + c^2 T$ provide the best description for $\rho/dT$ and $C_p$, respectively. We found an identical $\alpha \approx 0.2(2)$ in both $\rho/dT$ and $C_p$, as predicted by Fisher and Langer in a ferromagnetic metal. [2] These observations indicate strong critical scattering of conduction electrons by short-range spin fluctuations near $T_N$. In addition, the $S$ is strongly enhanced at low temperatures. The temperature dependence of $S$ above $T_N$ follows closely the formula $S/T \propto -lnT$, which suggests that quantum critical fluctuations [3] plays a role in enhancing the thermoelectric power on top of the classic critical fluctuations.


K1.00048 The Superconducting Phase Diagram of V3Si0.98X0.02, X=Ni, Mn, Co, Fe, Cu. M.D. ALMEIDA, C.P. OPEIL, Boston College, J.C. LASHLEY, J.L. SMITH, Los Alamos National Laboratory — We report on the results of AC Resistivity measurements of V$_{3}$(Si$_{0.98}$X$_{0.02}$) in the presence of a magnetic field, where the dopants include Ni, Fe, Mn, Co, and Cu. From this we see a clear shift in the superconducting critical temperature of the materials in response to increasing in field strength. Additionally, diammetry measurements provide information on the thermal expansion coefficients of these materials.


K1.00050 DFT Calculation of the Electronic Properties and EEL Spectrum of NiSi$_2$$^1$. ROBERTO NUÑEZ-GONZÁLEZ, Departamento de Matematicas, Universidad de Sonora, ARMANDO REYES-SERRATO, DONALD H. GALVAN, Centro de Nanociencias y Nanotecnologia, UNAM, ALVARO POSADA-AMARILLAS, Departamento de Investigacion en Fisica, Universidad de Sonora — In this work we present theoretical band structure, total and projected density of states (DOS), dielectric function and electron energy-loss spectrum (EELS) of NiSi$_2$. The calculations were carried out using the Full-Potential Linearized Augmented Plane Waves (FLAPW) method, within the Density Functional Theory (DFT) with the Local Density Approximation (LDA). Our theoretical EELS results are in excellent agreement with recent experimental findings, indicating that the main peak corresponds to a plasmon. Additional peaks in our calculations are identified as interband transitions (at 2.67 eV, 4.77 eV and 6.1 eV) associated to transitions between Ni d to Si p states, and low magnitude plasmons (at 1.3 eV and 4.02 eV).

$^1$APA acknowledges CONACYT-Mexico for financial support through project 24060. ARS is grateful to CONACYT Project 52927 and UNAM-PAPIIT IN107508.

K1.00051 Using Image Processing Techniques for Cluster Analysis, and Droplet Formation in Phase Separating Fluids. GREGORY SMITH, ANA OPRISAN, College of Charleston, JOHN HEGSETH, University of New Orleans, SORINEL OPRISAN, College of Charleston, CAROLE LECOUTRE, YVES GARRABOS, DANIEL BEYSENS, University of Bordeaux, France, COLLEGE OF CHARLESTON TEAM, UNIVERSITY OF NEW ORLEANS COLLABORATION, UNIVERSITY OF BORDEAUX COLLABORATION — A series of experiments in Phase Separating Fluids

K1.00052 Insights on copper coordination and reactivity of endonuclease EcoRI by ESR spectroscopy and modeling. MING JI — The cleavage of DNA by restriction endonuclease EcoRI is catalyzed by metal ions such as Mg$^{2+}$. However, Cu$^{2+}$ does not catalyze the cleavage of DNA by EcoRI. In order to understand the functional difference between Cu$^{2+}$ and Mg$^{2+}$ coordination of Cu$^{2+}$ in the EcoRI-DNA complex was clarified by ESR and MD simulation. There are two Cu$^{2+}$ components in the specific EcoRI-DNA complex. Each component has one N atom from histidine imidazole and one oxygen atom from the phosphate backbone of DNA coordinate to Cu$^{2+}$ based on the ESR experimental results. MD simulation further confirmed that the Ni atom of His114 imidazole and one oxygen atom from the phosphate backbone of DNA coordinate to Cu$^{2+}$. Difference in the coordination of Cu$^{2+}$ and Mg$^{2+}$ explains their different functional behaviors.

K1.00053 Twist Defect in an Imprinted Cholesteric Elastomer$^1$. PAOLA CASTRO-GARAY. Departamento de Investigación en Física, Universidad de Sonora, Hermosillo, México, JUAN ADRIAN REYES, Departamento de Física Química, Instituto de Física, Universidad Nacional Autónoma de México, D.F, México, ADALBERTO CORELLA-MADUEÑO, Departamento de Física, Universidad de Sonora, Hermosillo, Son., México — We have found that a chiral twist defect inserted in a cholesteric elastomer gives rise to circularly polarized localized modes of both handedness. This defect enhances the resonance mode amplitude whose handedness is opposite to the cholesteric helix for high cross-linked density. Complementarily, for low cross-linked density, the circular polarization opposite to helix cholesteric of the elastomer is decoupled with the defect mode so that the resonance mode disappears. Finally, the resonance mode of the circularly polarization of the same handedness to elastomer helix is maintained either, for high or low cross-linked density.

$^1$P. Castro-Garay acknowledges the support form CONACYT.
Meso-scale Harmonic Analysis of Homogenous Dislocation Nucleation. ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — Under sufficiently high load dislocations will be nucleated in perfect crystals. A typical scenario is the nano-indentation of a defect-free metal. An outstanding issue is the prediction of where and under what loads nucleation will occur. Many criteria have been put forward which address this question, some in terms of the local stress field, others in terms of the local tangent stiffness of the material. More recently it has been questioned whether a local criterion can be used at all [1]. We address the locality of the nucleation process via analysis of molecular dynamics simulations in terms of the vibrational eigenmodes of the mesoscale regions of the crystal for various model systems. [1] R.E. Miller and D. Rodney, J. Mech. Phys. Solids 56(4) 1203-1223, 2008.

MAGNETISM: OXIDES AND NANOSTRUCTURES —

The origin of the double-triangle hysteresis loops in ErFeO₃ near the low temperature erbium ordering transition L.T. TSYMBAŁ, O. Galkin Donetsk Physics & Technology Institute, YA. B. BAZALIY, University of South Carolina and Institute of Magnetism, Kyiv Ukraine, G.N. KAKAZEI, Universidade do Porto, Porto, Portugal and Institute of Magnetism, Kyiv Ukraine — Magnetic properties of an orthoferrite ErFeO₃ are determined by the iron and the rare-earth magnetic ions. Interactions between magnetic sub-systems of ErFeO₃ lead to a sequence of orientation phase transitions observed in this material. In this work hysteresis loops in single crystal ErFeO₃ samples were studied below the spin-rotation transition region, T < 80 K. Above and around the compensation point Tcomp = 46 K the hysteresis loops are rectangular, with the coercive force diverging at Tcomp. As the temperature is lowered towards the erbium ordering transition Tₓₓᵧᵧ = 4.1 K, the shape of the loops experiences a dramatic change. At 20 K the loops develop triangular “tails.” At 10 K the triangles become prominent while the central rectangular part near H = 0 collapses. A double-loop hysteresis pattern with two triangular loops emerges. We explain this behavior by a domain wall motion reversal mechanism with negligible pinning of the walls in the sample. The transition from the rectangular to the double-triangle loops is due to the competition between the energy barrier of wall nucleation and the demagnetization energy gain achieved by placing the wall inside the sample. Our model explains well the correlation of the loop’s shapes and sizes with the total magnetization of ErFeO₃.

Impact of transition metal buffer layers on Magnetite thin film growth and properties1, PRIYANGA JAYATHILAKA, DARYL WILLIAMS, CHRIS BAUER, DUSTIN BELJEY, CASEY MILLER, University of South Florida, Department of Physics — Magnetite thin films were grown on MgO single crystals with 3nm buffer layers of Fe, Cr, Mo, and Nb. An in situ masking system allowed the deposition of the individual buffer layers on separate substrates, followed by the simultaneous growth of 100nm thick magnetite films on all substrates via reactive sputtering. We are thus able to demonstrate the impact of the resulting lattice strain on the magnetite films’ structure, and temperature dependent resistivity and magnetization.

Origin of multiferroicity in hexagonal Y₁₋ₓDyₓMnO₃, A.K. SINGH, School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067 India, S.D. KAUSHIK, V. SRIRUGURI, UGC-DAE-CSR Mumbai Centre, Bhabha Atomic Research Centre, Mumbai 400085, India, S. PATNAIK, School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067 India — Multiferroic materials, that offer the possibility of manipulating an ordered electric state by applying magnetic field, have attracted considerable attention in the recent past. Here we report a detailed analysis of structural, magnetic and dielectric properties of polycrystalline samples of Y₁₋ₓDyₓMnO₃ (0 ≤ x ≤ 0.2). These materials belong to space group P6₃mc with hexagonal crystal structure and were synthesized by solid state reaction method. We have carried out extensive zero field and in-field neutron diffraction, and dielectric measurements. Our study provides evidence for change in the lattice parameters, buckling of Y (Dy) layers, Mn-O-Mn bond angles and tilting of MnO₆ polyhedra as a function of temperature and magnetic field. We also study the magnetoelectric coupling in YMnO₃ as well as doped samples by in-field dielectric measurements. A distinct anomaly near Néel temperature is observed in these measurements that vary with the application of magnetic field. In essence, we develop a model to understand the magnetoelectric coupling of these antiferromagnetic multiferroics with their field dependent magnetic structure.

Anomalous magnetic transition in multiferroic BiMnO₃ under high pressure, CHIH CHIEH CHOU, S. TARAN, J.L. HER, C.P. SUN, C.L. HUANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan, H. SAKURAI, A.A. BELIK, E. TAKAYAMA-MUROMACHI, Advanced Nano Materials Laboratory (ANML), National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan, H.D. YANG, Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan — The magnetic-field-dependent dc magnetization and the pressure-dependent (pmax ~ 16 kbar) ac susceptibilities χp(T) on both powder and bulk multiferroic BiMnO₃ samples, synthesized in different batches under high pressure, are reported. The ferromagnetic (FM) transition (Tc ~ 100 K) increases with higher magnetic field. The magnetic hysteresis shows the behavior as a soft ferromagnet. Ac susceptibility data indicate the following phenomena. (I) The FM peak (peak I) and its temperature (Tc) decrease simultaneously with increasing pressure. (II) Above a certain pressure (9 -11 kbar), another peak (peak II) appears at (Tc ~ 93 K). (III) Peak II also decreases with increasing pressure. (IV) Both these peaks persist over some intermediate pressure range (9-13 kbar). (V) Peak I disappears with further application of pressure; however, the second peak survives until present pressure limit (pmax ~ 16 kbar). These features are considered to originate from the complex interplay of the magnetic and orbital structure of BiMnO₃ being affected by pressure.

Magnetic frustration and spin glass behaviour in layered lithium oxide, LiNi₀.₆₅Co₀.₂₅Mn₁₀O₂, MAGNUS WIKBERG, PETER SVEDE LINDB, Dep. Eng. Sciences, Uppsala University, MOHAMMED DAHBI, ISMAEL SAADOUNE, ECME, LP2E2M, FST Marrakech, University Cadi Ayyad, PORTBORG JÖNS GUSTAFSSON, KRISTINA EDSTROM, Dep. of Materials Chemistry, Uppsala University — Samples of LiNi₀.₆₅Co₀.₂₅Mn₁₀O₂ with different amount of Li (x) have been investigated with ac and dc SQUID magnetometry, X-ray diffraction as well as with neutron scattering. The LiₓNi₀.₆₅Co₀.₂₅Mn₁₀O₂ exhibit a rhombohedral structure (space-group Rh3m) with non-magnetic Li⁺ layers alternating with transition metal (TM) slabs with edge-sharing oxygen octahedras. The nickel slabs contain several intralayer interactions of both antiferromagnetic (AFM), ferromagnetic (FM) type, e.g. 90° Ni₂⁺⁻Mn⁺⁺ and 90° Ni⁺⁻Ni⁺⁻, respectively. Also, the presence of Ni²⁺ in the Li-plane further induces AFM and FM couplings due to 180° superexchange interactions between Ni²⁺ ions in the Li-plane and TM⁺ ions present in the slabs. The resulting magnetic structure shows no evidence of long range order due to a high degree of spin frustration, thus yielding magnet properties reminiscent of a spin glass.

Spin and charge orderings in single layered cobaltate Laₓ−₁CaₓCoO₄ (0.3 < x < 0.8), KAZUMASA HORIGANE, HARUHIRO HIRAKA, TORU UCHIDA, KAZUYOSHI YAMADA, JUN AKIMITSU — Neutron scattering experiments were performed on single crystals of layered cobalt-oxides Laₓ−₁CaₓCoO₄ (LCCO) to characterize the charge and spin order in a wide hole-doping range of 0.35 ≤ x ≤ 0.8. For a commensurate value of x = 0.5 in (H,0,L) plane, two types of superlattice reflections concomitantly appear at low temperature; one corresponds to a checkerboard charge ordered pattern of Co²⁺/⁺ ions and the other is magnetic in origin. Further, the latter magnetic-superlattice peaks show two types of symmetry in the reflections, suggesting antiferromagnetic-stacking (AF-S) and ferromagnetic-stacking (F-S) patterns of spins along the c direction. From the hole-doping dependence, the in-plane correlation lengths of both charge and spin orders are found to give a maximum at x = 0.5. These features are the same with those of x = 0.5 in Laₓ−₁Srₓ+₁MnO₄ (LSMO), a typical checkerboard and spin ordered compound.
K1.00062 Electronegativity and Valence Electron Spectrum of Room Temperature Ferromagnets\(^1\) O. PAUL, ISIKAKU-IRONKWE, The Center for Superconductivity Technologies, Abuja FCT, Nigeria — Materials that exhibit room temperature ferromagnetism (RTFM) are of interest in the fabrication of spintronic devices. RTFM has been observed in semiconductors, oxides and other non-magnetic materials and nanocrystals. There is yet no consensus on the origin of RTFM or how to predict the next RTFM. Here we study the electronegativity and valence electron count of known RTFMs as a step to understanding this fascinating family of materials. Understanding the process of RTFM may aid the search for *room temperature superconductivity* (RTS) — a similar phenomenon.

\(^1\)Research support from ISEM, University of Wollongong, New South Wales 2522, Australia.

K1.00063 Molecular nanomagnets for information technologies\(^1\) MARCO AFFRONTI, CNR-INFN-S3 — I have recently reviewed challenges, achievements and perspectives in the field of molecular magnets in a review article in J. of Mat. Ch. DOI: 10.1039/b809251f (2008) focusing on quantum information. Molecular magnets are indeed quantum objects, with well-defined spin states at low temperature. The challenge is to obtain scalable quantum hardware with long coherence time. A paradigmatic case is that of AF rings in which an extra spin was introduced to have a S=1/2 as ground state (Phys. Rev. Lett. 94, 190501 (2005) and use excited states as a resource for implementing two-qubit gates (Phys. Rev. Lett. 94, 190501 (2005), Phys. Rev. B 76, 024408 (2007)). The mechanism of decoherence can be studied in details by considering hyperfine interactions with finite number of nuclear spins (Physical Review B 77, 054428 (2008). Cr7NI are stable in solution, can be functionalized to be grafted on surface (Inor. Chem. 46, 4968-4978 (2007) or to be linked each other by forming supramolecular complexes (Angew. Chem Int. Ed. 44, 6496 (2005) and Nature Nanotechnology 2008) with tuneable entanglement of spin states.

K1.00064 Correlation effects on the properties of small cobalt clusters\(^1\) YVETTE HANCOCK, MARI IJÄS, Department of Engineering Physics, Helsinki University of Technology, Finland — Demands for higher-density magnetic storage media and smaller memory devices require atomic-scale magnetic components with stable magnetic properties. One such candidate for this application is a small transition metal cluster. The magnetic properties of transition metal clusters are often strongly sensitive to the geometry of the cluster, the local atomic and structural environments, and to the system size. In this work, the GGA + U DFT method is used for the first time to study the system properties of small cobalt clusters consisting of 2 to 5 atoms. Previous studies using DFT and tight-binding approaches have been found to overestimate the binding energies, dissociation energies and vibrational frequencies of the clusters against their known experimental values. By including a Hubbard U correction between 2 – 3 eV, the DFT method can then be fitted to reproduce the experimental results, thereby improving upon previous theoretical descriptions of these systems. The effect of U on the calculated magnetic and structural properties of the clusters is also discussed.

K1.00065 Temperature and size dependence of electron magnetic resonance spectra of Ni nanoparticles chemically dispersed in silica\(^1\) VIVEK SINGH, MOHINDAR SEEHRA, West Virginia University — The temperature dependence (5K to 300K) of the electron magnetic resonance (EMR) lines observed at 9.28 GHz in Ni:SiO\(_2\) (15:85) nanocomposites with mean diameter D of the Ni nanoparticles (NPs) of D=3.8, 11.7, 15 and 21 nm are reported. The sizes of the Ni NPs were determined by TEM and XRD, with SiO\(_2\) being in the amorphous state. The procedures for the synthesis of the samples along with their DC and AC magnetization behavior were reported recently [1]. In EMR, three resonance lines are observed: (i) Line 1 with linewidth \(\Delta H \approx 50\) Oe and \(g \approx 2\), and Curie-like variation of the line-intensity, with \(\Delta H \approx H\) being temperature and size-independent; (ii) Line 2 with \(\Delta H \approx 950\) Oe and \(g \approx 2.2\) for \(D=3.8\)nm at 300K with both \(\Delta H\) and \(g\) increasing with decreasing \(T\) and \(\Delta H\) size-dependent; and (iii) weak line 3 with \(g \sim 4\) at 300K, with \(g\) also increasing with decreasing \(T\). We argue that the line 1 is due to dangling bonds in SiO\(_2\) as a similar line with \(\Delta H \approx 9\) Oe is also observed in SiO\(_2\) without Ni doping. Lines 2 and 3 are attributed to magnetic Ni NPs and large Ni clusters respectively whose anisotropy is both size and temperature-dependent [2], leading to the observed \(\Delta H\) and \(g\) values of the lines.


K1.00066 Synthesis and Characterization of Gd and Nd Nanoparticles\(^1\) DULCE G. ROMERO, PEI-CHUN HO, Department of Physics, Cal. State U., Fresno, SAEED ATTAR, Department of Chemistry, Cal. State U., Fresno — Due to the reduced dimensionality, nano-sized materials have physical properties significantly different from the bulk material, such as, superparamagnetic behavior, enhanced magnetization, and self-organization [1-3]. Nano-sized materials have great potential for technical applications, for example, magnetic information storage, imaging, medical devices, and magnetic refrigeration. In this report, we will present the growth and filtration of rare-earth Gd and Nd nanoparticles by the inverse micelle technique [4]. The results of the characterization of these clusters by X-ray diffraction, scanning electron microscope, and energy-dispersive x-ray spectroscopy will be presented.


K1.00067 Development of ferromagnetism in Pd nanoparticles with reduction in size\(^1\) MOHINDAR SEEHRA, JAMES RALL, West Virginia University, J. LIU, C. ROBERTS, Auburn University — Bulk fcc Pd is a paramagnet just missing the Stoner criterion for ferromagnetism (\(N(E_F)\| > 1\)) [1]. Several groups have reported weak ferromagnetism in 2-4 nm Pd nanoparticles (NPs) [2]. We report systematic development of weak ferromagnetism in Pd NPs with reduction in size. Magnetic measurements (\(M vs. T\)) are compared for bulk Pd with those of size \(D\) \(\approx 50, 70, 80\) and 60 nm. The samples of size \(D=7, 6, 5, 4, 3, 2, 1, 0\) and 6 mm were prepared by an aqueous seed-mediated growth and characterized by TEM and x-ray diffraction with the latter showing expansion of the lattice with decrease in size. Compared with the low-field magnetic susceptibility of bulk Pd, the 7 and 6 nm NPs are enhanced by an order of magnitude. For the 50 nm NPs, \(\chi\) follows nearly the Curie law. The hysteresis loops (\(M vs. H\)) for the 7 and 6 nm NPs shows a decrease in coercivity and remanence from 3K to 300K suggesting \(\Delta H > 300K\). Origin of this ferromagnetism in terms of surface magnetism and lattice expansion is discussed.


\(^1\)Research is supported by Fresno State start-up fund.

K1.00068 Mössbauer and magnetic studies of \((\text{Ni}_{0.6-x}\text{Co}_x)\text{Zn}_{0.4}\text{Fe}_2\text{O}_4\) nanoparticles\(^1\) J.C. HO, Wichita State University, M.M. EL-TABEY, Menoufia University, H.H. HAMDEH, R. ASMATULU, Wichita State University, S.H. WU, Y.Y. CHEN, Academia Sinica Mixed-ferrites (\(\text{Ni}_{0.6-x}\text{Co}_x)\text{Zn}_{0.4}\text{Fe}_2\text{O}_4\) with \(x = 0, 0.1, 0.2, 0.3, 0.4, 0.5\) and 0.6 were synthesized by co-precipitation of Ni-, Co-, Zn- and Fe-sulfates. Structural characterization of the approximately 10-nm particles was made by x-ray powder diffraction. Through Mössbauer spectroscopic measurements, the composition- and temperature-dependence of magnetic blocking temperature and anisotropic constant were obtained. SQUID data yielded corroborative results, in addition to magnetization and saturation values.
K1.00069 Effect of Anisotropy in Two-dimensional Dimer model of magnetic ferrofluids1. ABDALLA OBEIDAT, WESAM AL-SHARO, Jordan University of Science and Technology — The magnetization and the Initial susceptibility have been calculated using statistical mechanics for two-dimensional structured dilute ferro-fluid taking the effect of the magnetic anisotropy and inter-particle interaction. We assumed the assembly consists of N/2 non-interacting systems. Each system is composed of 2 interacting single domain fine magnetic spherical particles. We referred to this model as a Dimer-model. We found that when the easy axis is fixed with respect to the external magnetic field, the ordering temperature depend on the anisotropy constant K in both parallel and perpendicular cases.

1Jordan University of Science and Technology

K1.00070 Magnetic Nanoparticle Arrays prepared via Coaxial Electrospinning, NIKHIL SHARMA, HASSNAIN JAFFARI, ISMAT SHAH, DARRIN POCHAN, University of Delaware — One dimensional nanoparticle (1D NP) arrays display strong anisotropy in their physical properties making them interesting from a fundamental as well as applications perspective. 1D arrays of Fe3O4 nanoparticles have been constructed by encapsulating magnetite nanoparticles within Poly(ethylene oxide) nanofibers, by a modified solution spinning process. Electrospinning is a facile process for creating 1D nanostructures and a simple modification to the process renders a coaxial delivery mechanism that facilitates the construction of nanoparticle arrays. These hybrid 1D nanomaterials were structurally characterized by electron microscopy and the magnetic characteristics of these fiber encapsulated particle arrays were studied using vibrating sample magnetometry. Anisotropic magnetic behavior along different orthogonal axes (parallel and perpendicular) was observed even at room temperature with an appreciable increase in coercivity in the perpendicular configuration. Experimental work is underway to use these particle arrays as precursor materials for the creation of magnetite nanorods.

K1.00071 Initiating magnetization switching in computational Fe nanopillars via local heating, SAM THOMPSON, GREG BROWN, Florida State University, MARK NOVOTNY, Mississippi State University, PER RIKVOLD, Florida State University — The use of high-coercivity materials in recording media assists in extending the areal information density by allowing smaller, more closely spaced bits. To achieve densities greater than one terabit per square inch, however, the necessary coercivity of the particles challenges the maximum applied field that can be attained by the write head. One proposed technique to overcome this dilemma is heat-assisted magnetization reversal (HAMR), in which a locally applied heat pulse lowers the coercivity, allowing the applied field to initiate switching. To model this, we employ micromagnetic simulations of iron nanoparticles with thermal fluctuations that depend spatially and temporally on a solution of the heat equation corresponding to an initial heat pulse applied to the end of the pillar. For the case of an applied magnetic field parallel to the easy axis, the magnetization-switching behavior is explored as a function of total heat input and applied-field magnitude.

K1.00072 Fabrication of magnetic trilayer stripes using interference lithography, MENG ZHU, NIST, Gaithersburg, MD, 20899 / University of Maryland, College Park, MD, 20742, JAMES MACARTHUR, Swarthmore College, Swarthmore, PA, 19081, ROBERT MCMICHAEL, NIST, Gaithersburg, MD, 20899-8412 — Both theoretical (PRB, 74, 024424, 2006) and experimental (APL, 90, 232504, 2007) studies of a single layer magnetic film edge have shown that the edge-mode of magnetization precession detected by ferromagnetic resonance (FMR) is an effective tool to probe magnetic properties of thin film edges. To extend the measurement technique to realistic devices such as spin-valves or tunnel junctions, magnetic multilayer stripes have to be fabricated. Here, we present the fabrication of Py/Cu/Co magnetic trilayer stripes by interference lithography. A resist stack consisting of positive photoresist 1805 and WIDE-B anti-reflective coating (ARC) is exposed by a blue laser at 405nm using Lloyd’s mirror interferometer. Optimal soft-baking temperature of ARC results in an undercut during the development of the photoresist. This undercut facilitates the lift-off process after the evaporation of Py/Cu/Co trilayer. A uniform array of trilayer stripes with a period of ~620nm was obtained. This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement and NIST CNST-NSF REU #DMR-0754115.

K1.00073 Enhanced magneto-optical effect in two-dimensional spin photonic crystals, JINBAE KIM, WONCHANG NAM, NISHAD DESHPANDE, XINGRI JIN, MINSOO SEO, SUNG-JAE LEE, YOUNGPAK LEE, Hanyang University, Korea, JOOYULL RHEE, Sungkyunkwan University, Korea, KIWON KIM, Sungmoon University, Korea — Patterned arrays of magnetic nanostructures have become one of the key issues in recent years because of their potential application to the information technology which utilizes optical and magnetic storage devices. In this study, we have successfully fabricated two-dimensional patterned arrays of Co by using the photolithography and the wet-etching process. The magnetic anisotropy, the magnetic domain structures, and the magnetization reversal process are investigated by means of magnetic-force microscopy and magneto-optical Kerr effect. The in-plane magnetization reversal process could be understood through a detailed investigation the field-dependent magnetic domain structures. The magneto-optical response is measured for both reflected and diffracted beams, and compared with the results of micromagnetic simulation.

K1.00074 Fabrication and characterization of rectangular thin film planar loops for transformer applications, GREGORY A. TOPASNA, DANIELA M. TOPASNA, FRANK R. POWELL, Virginia Military Institute — This study focuses on optimizing the configuration and performance of a thin film planar loop that is flux linked to a short straight wire. Our calculations for the mutual inductance show its dependence on the geometry of the planar loop as well as on its location relative to the wire. We have fabricated and characterized various geometries and compared the data to the solutions predicted by our model. These results are used in designing the next generation of devices which will incorporate magnetic nanoparticles.

K1.00075 MAGNETISM: DYNAMICS AND TRANSPORT —

K1.00076 Laser-induced orbital and spin excitations in ferromagnets: Insights from a two-level system1, GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, Indiana 47809, YIHUA BAI, Center for Instruction, Research and Teaching, Indiana State University, Terre Haute, Indiana — A recent element-specific and time-resolved measurement in Fe/Gd multilayers showed the laser-induced orbital and spin excitations proceed in unison and the spin-orbit ratio is held constant during the demagnetization. Here a two-level model shows that these orbital and spin excitations originate from state population and state interference effect. For an addressed state, spin and orbital dynamics are solely from the state interference, where the spin and orbital momenta oscillate with the laser frequency and match the dipole moment exactly, an unambiguous test case for time-resolved magneto-optical Kerr effect. For an undressed state, the inference effect introduces a rapid beating in orbital momentum, which is observed in the first-principles calculation in fcc Ni. The state population change leads to a constant spin-orbit ratio, which explains the linear dependence between spin and orbital momentum changes within 2 ps upon the arrival of pump pulse in ferromagnetic iron.

1Supported by DOE under Contract No. DE-FG02-06ER46304, Promising Scholars grant, and NERSC at LBNL under Contract No. DE-AC02-05CH11231.
K1.00077 Origin of light-induced precession of magnetization in ferromagnetic (Ga,Mn)As. 
EVA ROZKOTOVA, PETR NEMEC, DANIEL SPRINZL, NADA TESAROVA, PETR MALY. Charles University in Prague, Ke Karlovu 3, 121 16 Prague 2, Czech Republic, VIT NOVAK, KAMIL OLEJNIK, JAN ZEMEN, MIROSLAV CUJKR, TOMAS JUNGWIRTH, Institute of Physics ASCR v.v.i., CuKovnická 10, 162 53 Prague, Czech Republic, JOERG WUNDERLICH, Hitachi Cambridge Laboratory, Cambridge CB3 0HE, United Kingdom — The impact of femtosecond laser pulse leads to the precession of magnetization in (Ga,Mn)As, which can be detected by the time-resolved Kerr rotation (KR) technique. Even though this phenomenon is known for several years [1], the exact physical mechanism inducing the precession is still not clear [2,3]. We show, by a detailed comparison of the KR experimental results and the microscopic calculations of the magnetic anisotropy, that the precession is a consequence of the anisotropy field modification due to the laser pulse-induced change of hole concentration and lattice temperature. [1] A. Oiwa, H. Takechi, H. Munekata. J. Supercond. 18, 9 (2005).[2] Y. Hashimoto, S. Kobayashi, H. Munekata, PRL 100, 067202 (2008).[3] E. Rozkotova, P. Nemec, P. Horodyiska, D. Sprinzel, F. Trojane, P. Maly, V. Novak, K. OleJNIK, M. CuK, T. Jungwirth, Appl. Phys. Lett. 92, 122507 (2008).

K1.00078 Longitudinal Field µSR Study of Spin Dynamics and Onset of Magnetic Correlations in LiY_{1-x}Ho_{x}F_{2} with 0.002 ≤ x ≤ 0.101. R.C. JOHNSON, K. CHEN, M.J. GRAF. Department of Physics, Boston College, Chestnut Hill, MA 02467 USA — The Ho^{3+} ions in LiY_{1-x}Ho_{x}F_{2} exhibit a crossover from single ion to spin glass behavior with increasing x. We have studied the longitudinal field depolarization rate for samples with 0.002 ≤ x ≤ 0.10 over the temperature range 50 mK ≤ x ≤ 50 K and for magnetic fields up to 0.1 T. For low concentrations, we find a peak in the temperature-dependent depolarization, as often observed in 1/T1 NMR measurements on single molecule magnets (SMM); at high concentrations the depolarization rate increases monotonically with decreasing temperature. These results suggest that the difference in behavior of SMMs systems as seen in NMR and µSR measurements may be due to differences in the strength of the interactions between the magnetic clusters.

1Supported by National Science Foundation grant DMR-0710525.

K1.00079 A $^{51}$V NMR Investigation of the Quasi-1D Antiferromagnet BaCo_{5}V_{2}O_{14}: Is there a New ordered Phase?. T. BESARA, Department of Chemistry, Florida State University, Tallahassee, FL, USA, L.L. LUMATA, Department of Physics, Florida State University, Tallahassee, FL, USA, K.-Y. CHOI, Department of Physics, Chung-Ang University, Seoul, Republic of Korea, A.P. REYES, P.L. KUHNS, National High Magnetic Field Laboratory, Tallahassee, FL, USA, N.S. DALAL, Department of Chemistry, Florida State University, Tallahassee, FL, USA, J.S. BROOKS, H.D. ZHOU, C.R. WIEBE, Department of Physics, Florida State University, Tallahassee, FL, USA — We report on detailed $^{51}$V (I=7/2) NMR spectral and spin-lattice relaxation time (T1) measurements on the quasi-1D antiferromagnet BaCo_{5}V_{2}O_{14}. Our major focus was on probing the possible existence of the new ordered state in its field-induced phase above the critical field H_{c}. This phase is believed to be of the incommensurate type, and thus quite amenable to investigation by NMR line shape and T1 measurements. T1 data were obtained using a spin-echo pulse sequence. Measurements were done on a single crystal, with the field parallel to the easy axis (c-axis). Details of the lineshape and T1 analysis in terms of the evolution of the anticipated new phase will be presented.

K1.00080 NMR and Spin Relaxation in Systems with Magnetic Nanoparticles: Effects of Size and Molecular Motion, NATALIA NOGINOVA, TRACEE WEAVER, NSU, Norfolk, VA, ALEXANDR ANDREYEV, Virginia Tech, Blacksburg, VA, VADIM A. ATSARKIN, IRE, Moscow, Russia — To better understand the specifics of nuclear magnetic resonance and spin relaxation in systems with magnetic nanoparticles and test the limits of the outer sphere model for the diffusion related relaxation, iron oxide nanoparticle suspensions were studied in the dependence of the particle size, and for different degree of molecular motion. For the liquid suspensions with relatively small particles or clusters, spin relaxation rates well correspond to the theory, which predict maximum and decrease of the longitudinal rate and increase in the transverse rate with the increase in the effective radius, R. For the larger particle size > 20 nm, as well as in cases of strong aggregation or slowdown of molecular motion, the relaxation rates are significantly lower than theoretical predictions. We discussed the results and frames of the fast-motion and fast-diffusion approximations.

K1.00081 Magnetic properties of MnCrO_{4} investigated by NMR. DONG YOUNG YOON, SOONCHIL LEE, Department of physics, Korea Advanced Institute of Science and Technology, YOON SEOK OH, KEE HOON KIM, Department of physics and astronomy, Seoul National University — We investigated the magnetic properties of spinel MnCrO_{4} by nuclear magnetic resonance (NMR) and superconducting quantum interference device (SQUID). The magnetization vs. temperature curves under zero field cooling and field cooling show the ferrimagnetic spiral structure below 20 K and the collinear ferrimagnet from 40 K to 20 K. The magnetization vs. time curve show the spin-glass-like behavior below 9 K. The canting angles of Mn and Cr spins at liquid He temperature are determined by NMR to be 50° and 110°, respectively. In the ferrimagnetic spiral state, the nuclear spin-spin relaxation rate steeply increases with increasing temperature above 12 K, which expected to come from the fast fluctuation of electron spins. The NMR shows that the volume of the ferrimagnetic spiral domain decreases faster than the local magnetization as temperature increases. Furthermore, the domain volume shows the differences between cooling and warming processes. We depict that the ferrimagnetic spiral is embedded in the collinear ferrimagnet matrix.

K1.00082 Direct Observation of Orbital Reorientation in MnV_{2}O_{4} by NMR. JEONG HYUN SHIM, EUNA JO, JOOSEOEP LEE, SOONCHIL LEE, Department of Physics, Korea Advanced Institute of Science and Technology, DAEJONG 305-701, KOREA, TAKEHITO SUZUKI, TAKUYO KATSUFUJI, Department of Physics, Waseda University, Tokyo 169-8555, Japan — The effect of magnetostriction on the orbital states on the MnV_{2}O_{4} was investigated by rotating the direction of magnetic field. The microscopic evidence of the orbital reorientation process, induced by the rotation, was found from the variation of V^{3+} NMR spectrum. Despite the magnetic field is rotated from z axis to y axis, NMR spectrum of 0° is almost identical to that of 90°, which reveals the reorientation of the orbital states of V^{3+} ions following deformation of lattice. It was also observed that the reorientation process takes place suddenly when the magnetic field made 45° with respect to the z axis. Such a sudden behavior implies that the orbital-lattice coupling is much stronger than the spin-orbital coupling in MnV_{2}O_{4}.

K1.00083 In-plane and out-of-plane ferromagnetic resonance investigations of epitaxial CrO_{2}(110). HWACHOL LEE, KRISHNA CHETRY, CLAUDIA MEWES, ARUNAVA GUPTA, TIM MEWES. The University of Alabama — We report on in-plane and out-of-plane ferromagnetic resonance experiments to determine the magnetization damping in epitaxial CrO_{2}(110) thin films. The films were grown on TiO_{2} (110) substrates using chemical vapor deposition (CVD) with a CrO_{3} precursor [1]. Ferromagnetic resonance experiments as a function of the in-plane angle confirm a uniaxial in-plane anisotropy with the easy axis aligned parallel to the in-plane easy axis of the film and along the film normal. Both measurements show a weak dependence of the linewidth on the microwave frequency once the sample is fully saturated. The effective damping constant as determined by the frequency dependent measurements is very small. Over the experimentally accessible frequency range (4-60 GHz) the dominant contribution to the ferromagnetic resonance linewidth is therefore extrinsic in nature. References: [1]: X. W. Li, A. Gupta, and G. Xiao, Appl. Phys. Lett. 75, 713 (1999).

3We gratefully acknowledge support from the NSF (DMR 0804243).
EID, Miami University — We have measured the contact resistance between the ferromagnetic semiconductor GaMnAs and each of the metals silver, aluminum, and copper. We have observed giant positive magnetoresistance with its saturation field increasing with increasing temperature, which is well explained by the Zeeman splitting of the localized states that suppresses the spin dependent hopping paths in the presence of magnetic field.

This work is supported by the NSF DMR-0547036.

K1.00085 Excitations in the chiral spin liquid

DARRELL SCHROETER, Reed College — Recently, a spin-Hamiltonian was presented [Schroeter et al., Phys. Rev. Lett. 99, 097202 (2007)] for which the chiral spin liquid is the exact ground state. This poster will present a numerical study of the excitations of the model, including results obtained by exact diagonalization of the model on 16 and 25-site lattices.

K1.00086 Electrical and Optical Characterization of Spin Transfer Torques

JOSHUA EMERICK, S.C. PARKS, K. LI, A. HAUSER, J. E. THOMPSON, J. CIRALDO, J. LUCY, F. Y. YANG, E. JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — The spin-transfer torque (STT) phenomenon is a direct outgrowth of giant magnetoresistance (GMR) in the regime of high current density. Investigations of this phenomenon have contributed to improved understanding of fundamental processes and revealed the potential for technological innovation. To further this exploration, we have constructed an instrument that simultaneously measures microwave electrical response and magnetization in an external magnetic field of up to 1 T. The microwave probe is sensitive at frequencies up to 30 GHz and the magneto-optical Kerr effect (MOKE) magnetometer is configured to measure the magnetization of the active region during operation (resolution of ~ 100 µm). We present the experimental configuration of this instrument and calibration data from prototype samples. The ability to directly measure layer orientation for active devices provides a powerful tool for the investigation of STT.

Partial support for this research provided by the OSU Institute for Materials Research and NSF ECCS Grant No. 0726133.

K1.00087 Pure Spin Current Injection through Superconductive/Normal Metal Ohmic Interface

KOHEI OHNISHI, ISSP University of Tokyo, TAKASHI KIMURA, YOSHICHIKA OTANI, ISSP University of Tokyo, ASI RIKEN — In past few years, spin-dependent transport properties in nano-structured systems have drawn considerable attention owing to potential applications in spintronics. Spin transport has so far been investigated both experimentally and theoretically much more intensively in normal- or semi-conductors than in superconductors. However recent theoretical studies on the spin transport in superconductor predict the intriguing phenomena such as the non-linearity and the control of superconductivity that may lead to functional superconductive spintronic devices. Therefore, it is urgent to elucidate experimentally the spin transports in superconductor. Here, we investigate the influence of pure spin currents on superconductivity in a lateral structure consisting of superconductive Nb, normal metal Cu and ferromagnetic Ni-Fe wires. Using nonlocal spin injection technique, we found that pure spin current injection into the superconductive Nb wire induces the voltage drop along the wire. This can be understood as conversion from the spin current to the supercurrent via the quasi-particle current.

K1.00088 Spin-dependent conductance switching in organic molecular junctions

YUN-WEN CHEN, LUIS A. AGAPITO, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — We use density-functional theory to calculate the electronic transport through single molecules attached to capped (5,5) carbon nanotubes (CNT's) as leads. We observed a strong variation in the electrical conductance with respect to the spin-state of the junction. The singlet state exhibits high conductance whereas the triplet low. The deformation of the CNT's cap structure, upon covalent adsorption of the phenyl rings, triggers the spin dependence in the organic junctions. Two different π-conjugated phenylene-vinylene-containing molecules were tested, yielding similar behavior.

Acknowledgement: this work is supported by the DOE under Grant No. DE-FG02-02ER45995.

K1.00089 Giant positive magnetoresistance in Co@CoO nanoparticle array

HUI XING, WENJIE KONG, CHAEHYUN KIM, University at Buffalo-SUNY, SHOUHENG SUN, Brown University, ZHUAN XU, Zhejiang University, HAO ZENG, University at Buffalo-SUNY — The spin-dependent charge transport has been extensively studied due to its technological applications in information industry. Of particular interests are magnetic granular systems consisting of magnetic grains embedded in a nonmagnetic matrix, which typically exhibits negative granular MR. Interestingly, anomalous positive MR in granular systems has been reported in different materials [1]. Possible origins that can account for the positive MR include: ordinary MR caused by the curvature of the carrier trajectories in the magnetic field, shrinkage of the wave functions of localized electronic states due to the external field, and suppression of hopping paths due to the Zeeman splitting of the localized state. Here we present magnetotransport studies in self-assembled Co@CoO nanoparticle arrays which provide model granular systems. Efros Shklovskii variable range hopping to Mott variable range hopping crossover occurs at around 25 K. Giant positive MR with its saturation field increasing with increasing temperature is observed, and is well explained by the Zeeman splitting of the localized states that suppress the spin dependent hopping paths in the presence of magnetic field.


Research supported by NSF DMR-0547036.

K1.00090 ABSTRACT WITHDRAWN

K1.00091 Measurements of the Contact Resistance Between GaMnAs and Different Metals

NOAH OPOONDO, GRANT RILEY, ROBERT TOLLEY, TYLER BREST, Miami University, XINYU LIU, JACEK FURDYNA, Notre Dame University, KHALID EID, Miami University — We have measured the contact resistance between the ferromagnetic semiconductor GaMnAs and the metals, yet the very high carrier concentration in GaMnAs causes the contact resistance to be quite small and ohmic. We will also discuss the possible mechanisms of conduction at the interface. Determining the contact resistance of GaMnAs is important for spin injection experiments. This work is supported by the Research Corporation for Science Advancement.

K1.00092 Vortex-core reversal by rotating currents , THOMAS KAMIONKA, MICHAEL MARTENS, MARKUS BOLTE, GUIDO MEIER, Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Germany, KANG WEI CHOU, TOLEK TYLISZCZAK, Advanced Light Source, LBNL, Berkeley, CA, USA, MICHAEL CURCIC, BARTEL VAN WAENENBERGE, HERMANN STOLL, Max Planck Institute for Metals Research, Stuttgart, Germany — The investigation of the interaction between a spin-polarized current and the magnetization of a ferromagnet is of great interest. One concept for data storage is to use the current-induced switching of the vortex-core polarization, i.e. the out-of-plane component of the magnetization in the center of a micromized permalloy element. It has been shown both theoretically [1] and experimentally [2] that the polarization can be switched selectively by resonant field excitation. We carried out time-resolved scanning transmission X-ray microscopy while exciting the vortex core with rotating currents of varying frequency, amplitude and rotation sense. We observed vortex core switching, and by analyzing the gyration phase with respect to the exciting current we derive whether the Oersted-field or the spin torque mainly contributes to the excitation and causes the switching process. [1] S. K. Kim et al., Appl. Phys. Lett. 92, 022509 (2008). [2] M. Curcic et al., Phys. Rev. Lett. 101, 197204 (2008).

K1.00093 Antivortex-core switching as write process in random access memories , ANDRE DREWS, TORU MATSUYAMA, LARS BOCKLAGE, MARKUS BOLTE, GUIDO MEIER, Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Germany, BENJAMIN KRUEGER, STELLAN BOHLENS, Institute of Theoretical Physics, University of Hamburg, Germany — Magnetic vortices observed in ferromagnetic thin films have received a great deal of interest in recent years. The topological counterpart of a vortex, the antivortex, has not been investigated as intensively so far. Like vortices, magnetic antivortices gyrate when excited by alternating fields or spin-polarized currents. When excited by alternating currents and fields simultaneously, the superposition of the forces leads to an enhancement or suppression of the gyration amplitude, depending on the orientation of the in-plane magnetization, i.e. the c-value of the antivortex, and the antivortex-core polarization p. Thus the c-p-dependent amplitude variation of antivortex core gyration can lead to antivortex-core switching and thus to write binary data. Reading out of the data can be done by detecting the amplitude of gyration, e.g. by inductive loops. A logical zero (one) is represented by a small (large) gyration amplitude, i.e., suppression (enhancement) of the gyration. Due to the c-p-dependence of the excitation amplitude, an ensuing toggle switching is impossible. This technique allows bringing the antivortex into a distinct binary state without the need of a reading process before writing the bits.

K1.00094 MAGNETISM: GENERAL AND THEORY –

K1.00095 Local hyperfine field systematic of sp impurities on (001) and (111) Ni Surfaces , MARCUS TOVAR COSTA, Universidade do Estado do Rio de Janeiro, Instituto de Aplicacaoo, Brazil, ALEXANDRE DE OLIVEIRA, Centro Federal de Educacao de Quimica de Nilopolis, Brazil — A self-consistent calculation of the local magnetic moments and the hyperfine fields is performed, considering a systematic of n-sp, (n=4,5) impurities on (001)Ni and (111)Ni surfaces and sub-layers. A simple model is adopted which is, in principle, an extension on that of Daniel and Friedel. The behavior obtained for the hyperfine fields for each one of the series namely above is drastically different from that obtained for the bulk. The calculations of the electronic structure of the systems are based on a full multi-orbital tight-binding model and using the Green function formalism. The effect of next-neighbor perturbation on the magnetic properties, due to the lost of translational invariance introduced by the impurity, is taken into account in the present picture. The theoretical results are in agreement with known experimental data.

K1.00096 Long-range behavior of exchange bias in CoFe/FeMn-based multilayers , NAM DAO, Department of Materials and Engineering, University of Virginia, WEI CHEN, Department of Physics, University of Virginia, KEVIN WEST, DAVID KIRKWOOD, JIWEI LU, Department of Materials and Engineering, University of Virginia, STUART WOLF, Department of Materials and Engineering and Department of Physics, University of Virginia — CoFe/FeMn-interface-based multilayers were grown in magnetic field and at room temperature. The exchange bias field $H_{EB}$ depends strongly on the order of depositions and is much higher for CoFe/FeMn than FeMn/CoFe bilayers. By combining the two bilayer structures into symmetric CoFe/FeMn ($f_{pMn}$)/CoFe trilayers, $H_{EB}$ is enhanced for both the top and bottom CoFe layers. Enhancements of exchange bias are also observed by reducing the FeMn thickness $t_{pMn}$ of the trilayers. These results evidence the propagation of exchange bias between the two CoFe/FeMn and FeMn/CoFe interfaces mediated by the FeMn antiferromagnetic order. Furthermore, the exchange bias is even considerably increased when a thin Al or Mg layer is inserted into the CoFe/FeMn interface (i.e., CoFe/Al/FeMn or CoFe/Mg/FeMn) and persists for the insertion layer thicknesses of up to about 1.5 nm. These results strongly indicate that exchange bias is not a pure interfacial phenomenon, but mainly governed by possible long-range couplings such as dipole-dipole and RKKY between the antiferromagnetic uncompensated spins and the ferromagnetic layer.

K1.00097 Direct Measurement of the Bose-Einstein Condensation Universality Class in NiCl$_2$-4SC(NH$_2$)$_2$ at Ultralow Temperatures$^1$, LIANG YIN, J.S. XIA, N.S. SULLIVAN, Department of Physics, University of Florida, and NHHMF, V.S. ZAPF, NHMF, Los Alamos National Laboratory, A. PADUAN-FILHO, Universidade de Sao Paulo — In this work, we demonstrate field-induced Bose-Einstein condensation (BEC) in the organic compound NiCl$_2$-4SC(NH$_2$)$_2$ using ac susceptibility measurements down to 1 mK. The Ni S=1 spins exhibit 3D XY antiferromagnetism between a lower critical field $H_{c1} \sim 2$ T and a upper critical field $H_{c2} \sim 12$ T. The results show a power-law temperature dependence of the phase transition line $H_{c1} (T) - H_{c1} (0) \approx \alpha T^\gamma$ with $\alpha = 1.47\pm 0.0$ and $H_{c2} (0) = 2.05 T$, consistent with the 3D BEC universality class. Near $H_{c1}$, a kink was found in the phase boundary at approximately 150 mK.$^1$This work was supported by NSF Cooperative Agreement No. DMR 0654118, the Department of Energy and the State of Florida, the Brazilian Agencies CNPq and FAPESP.

K1.00098 Magnetization Plateau of Classical Ising Model on Shastry-Sutherland Lattice$^1$, MINGCHE CHANG, National Taiwan Normal University, MIN-FONG YANG, Tunghai University — Magnetization of the classical antiferromagnetic Ising model on the Shastry-Sutherland lattice is investigated using the tensor renormalization group approach. We find a single magnetization plateau at 1/3 of the saturation value and investigate its dependence on temperature and frustration. The spin configuration of this plateau has also been determined.$^1$Supported by the National Science Council of Taiwan

K1.00099 Phase transitions in site diluted systems of Ising dipoles , JUAN J. ALONSO, Universidad de Malaga, JULIO F. FERNANDEZ, ICMA, CSIC-Universidad de Zaragoza — By Monte Carlo simulations, we study dilute systems of Ising magnetic dipoles on simple cubic lattices. Dipoles are restricted to point along the z axis and are randomly placed in a fraction $x$ of the $L^3$ sites of the lattice. For $x_c \approx 0.6$ we find a thermally driven second order transition between a paramagnetic and a dipolar antiferromagnetic (AF) phase at a temperature $T_{c}$ which can be fitted by $k_BT_{c}/E_g \approx 4.3(x-x_c)^{0.6}$, where $E_g$ is a nearest neighbor dipole-dipole interaction energy. We explore whether an equilibrium spin glass phase exists for $x < x_c$. To this end, we study the spin glass overlap parameter $q$ between equilibrium configurations which we obtain from tempered Monte Carlo simulations for systems of $N$ dipoles in the range $40 \leq N \leq 500$. For $x < x_c$ we find no AF phase transition. However, we observe rather large AF correlations at low temperatures for $0.2 < x < x_c$. For $x = 0.35, 0.5$ and 0.6 and temperatures below $k_BT/T_{c} \approx 0.9$ we find double-peaked distributions of $q/\langle q^2 \rangle^{1/2}$. Their shape does not change appreciably with $N$. For smaller values of $x$, for which previous results exists, we have not been able to obtain clear cut results.
K1.00100 Ab-Initio Study of Magnetic Properties of M-doped (M = Cr or V) ZnGeN\textsubscript{2} \textsuperscript{1} — J. RUFINUS, Science Division, Widener University, Chester, PA 19013 — The current interest in the emerging field of semiconductor spintronics is mostly focused on transition metal-doped binary materials. Recently, however, the explorations of transition metal-doped ternary semiconductors have intensified, due to some experimental confirmations of high Curie temperature in chalcopyrite compounds. In ternary materials, there are possibilities of having ferromagnetic or antiferromagnetic configurations, depending on which metal site was substituted by the dopant. A donor (i.e. releasing electrons) will be produced when a metal atom substitutes a lower valent site, while an acceptor (i.e. releasing holes) will be produced when a metal atom substitutes a higher valent site. Only holes are expected to lead to ferromagnetism. A density functional theory within generalized gradient approximation study was performed on M-doped (M = Cr or V) ternary material ZnGeN\textsubscript{2}. The objective of this study is to determine whether substitutional transition metal in a group II (Zn) site and in a group IV (Ge) site will be ferromagnetic or antiferromagnetic. Our results show that both Cr- and V-doped ZnGeN\textsubscript{2} to be ferromagnetic, independent of the substitution sites. Additionally, formation of half-metallic ferromagnetism is possible in this type of material.

\textsuperscript{1}Work supported by NSF, Teragrid, and Widener University Grants

K1.00101 Spin-glass transition of magnetic dipoles with random anisotropy axes \textsuperscript{4} — JULIO F. FERNANDEZ-DEZ, ICMA, CSIC-Universidad de Zaragoza, JUAN J. ALONSO, Universidad de Malaga — We study partially occupied lattice systems of classical magnetic dipoles which point along randomly oriented axes. Only dipolar interactions are taken into account. From Tempered Monte Carlo simulations, we obtain equilibrium results for xL\textsuperscript{3} dipoles, randomly located on L\textsuperscript{3} simple cubic lattice sites, for L = 4, 6, 8 and 12, with an x = 0.35, 0.5 and 1 fraction of occupied sites. The numerical evidence we obtain supports the existence of an equilibrium spin glass phase below a transition temperature T\textsubscript{SG}, given by k\textsubscript{B}T\textsubscript{SG} = \langle 0.9 \pm 0.1 \rangle x \epsilon d, where \epsilon d is a nearest neighbor dipole-dipole interaction energy. The spin glass overlap parameter q is statistically distributed, and its mean square deviation follows the rule, \langle q^2 \rangle \approx 0.25 \langle q \rangle^2 \langle x \rangle in the spin-glass phase.

K1.00102 A Finite Temperature First-Principles Model for Spin Fluctuations \textsuperscript{5} — YI WANG, SHUNLI SHANG, LONG-QING CHEN, ZI-KUI LIU — In the past decades, the steady increasing in both computer power and the efficiency of computational methods has made it realistic the accurate first-principles calculations of material properties at finite temperature. The current frontier is how to extend the first-principles approach when it becomes important of the role of the internal degrees of freedom, which is beyond the spatial degrees of freedom of a material. One of important examples is the interplay between magnetic and lattice fluctuations at finite temperature. Solution of this enigma can reveal the microscopic origin of the novel properties of many materials. Hereby we propose a general framework to calculate the Helmholtz energy for system with spin fluctuations. The theory has been applied for EuTiO\textsubscript{3}. The energetics includes 256 spin configurations, of a 2x2x2 supercell, which are reduced to 14 not equivalent ones. We find a Schottky anomaly in the specific heat at T = 5.8 K which is matching closely to the Neel Temperature of 5.5 K for EuTiO\textsubscript{3}.

K1.00103 Study of the magnetic structures of the atacamite and botallackite forms of Cu\textsubscript{2}(OH)\textsubscript{3}Cl in terms of first principles DFT calculations \textsuperscript{6} — JINHEE KANG, CHANGHOON LEE, MIKE H. WHANGBO, Department of Chemistry, North Carolina State University — The atacamite and botallackite forms of Cu\textsubscript{2}Cl(OH)\textsubscript{2} are made up of edge- and corner-sharing Cu(OH)\textsubscript{2}Cl\textsubscript{2} octahedra. Each polymorph consists of two slightly different types of Cu\textsubscript{2}Cl\textsubscript{2} octahedra, with their Cu\textsuperscript{2+} magnetic orbitals contained in the Cu(OH)\textsubscript{2} square planes. Atacamite and botallackite are different in the way the Cu(OH)\textsubscript{2} square planes are connected, but their magnetic properties of atacamite and botallackite are quite similar. To explain these observations, the crystal structures of the two polymorphs were optimized by first principles DFT calculations. We then evaluated the spin exchange interactions of the two polymorphs using the optimized structures on the basis of DFT calculations. To a first approximation, both polymorphs were found to be described by a uniform 1D antiferromagnetic chain model with spin frustration arising from the next-nearest-neighbor interactions. Implications of these observations were explored.

\textsuperscript{6}DMSE, OBES, and DOE

K1.00104 Electromagnetic response of the planar metamaterial consisting of cut-wire pair and continuous wire \textsuperscript{7} — VU DINH LAM, NGUYEN THANH TUNG, JINWOO PARK, SEONGJAE LEE, YOUNGPAK LEE, Hanyang University, Korea — The left-handed materials (LHMs) attract more and more attention in recent years because of their intriguing physical properties and applications. Recently, a simple structure, the so-called cut-wire pair (CWP) was proposed and successfully used as the magnetic component in fabricating the LHMs. The simple geometry of CWPs means that such structures can be scaled down to the nanometer dimension much more easily than those based on the conventional split-ring resonator structures. In addition, the main advantages of the CWP structure comparing to the other structures is its ability to produce a strong magnetic resonance for the normal-to-plane propagation with only one CWP layer. In this report, we present the influence of lattice constants on the electromagnetic properties of CWP structures in the microwave frequency regime. In addition, we also discussed on how the lattice constants affect the LH behavior of combined structure consisting of CWP and continuous wire. A good agreement between the measurement and the numerical simulation is achieved.

K1.00105 Magneto-optical imaging of magnetic domain pattern produced by intense femtosecond laser pulse irradiation \textsuperscript{8} — JAIVARHAN SINHA, SHYAM MOHAN, S.S. BANERJEE, Department of Physics, Indian Institute of Technology, Kanpur-208 016, U. P., India, S. KAHALY, G. RAVINDRA KUMAR, Tata Institute of Fundamental Research, 1 Homi Bhabha Road, Mumbai- 400 005, India — An important and intriguing area of research is laser plasma generated giant magnetic field pulses. Interaction of ultrashort high intensity laser pulses with matter involves several mechanisms for generating ultrastrong magnetic fields. By irradiating a magnetic recordable tape constituting of Fe\textsubscript{3}O\textsubscript{4} particles with an intense p-polarized femtosecond laser pulses (\sim 10\textsuperscript{16} W cm\textsuperscript{-2}, 100fs), we have found complex magnetic field patterns stored in the tape. We image the local magnetic field distribution around the irradiated region \textsuperscript{1} using the high sensitivity magneto-optical imaging technique. We understand the complex magnetic domains patterns recoded on the tape in terms of interesting instabilities \textsuperscript{1} generated in the plasma produced during the irradiation of the tape with intense laser pulses.\textsuperscript{1}

\textsuperscript{8}Jaivardhan Sinha, Shyam Mohan, S. S Banerjee, S. Kahaly, G. Ravindra Kumar, Phys. Rev. E 77, 046118(2008), *srayaji@itik.ac.in

K1.00106 INSTRUMENTATION AND MEASUREMENT SCIENCE —

K1.00107 Low Temperature Conducting Probe Microscopy of Carbon Nanotubes — IVAN BORZENETS, HENOK MEBRAHTU, ULAS COSKUN, MATTHEW PRIOR, GLEB FINKELSTEIN, Duke University Physics — In order to measure local electrical properties of nano-devices at liquid He temperatures, we have built an atomic force microscopy. The instrument is outfitted with a conducting tip, which allows us to acquire both topography and electrical signals at the same time. The AFM has a scan window of up to 10 microns at low temperature and allows one to translate the sample laterally by up to a millimeter. To find a specific device within this range, the samples structure has to be specially optimized by addition of the "search pattern". The electrically conducting tip of the AFM allows us to make a variety of measurements such as: gating and tunneling, and to apply a mechanical force to the sample.
K1.00108 Fabrication Of Nickel-tipped Cantilevers for Magnetic Resonance Force Microscopy, STEVEN HICKMAN, E.W. MOORE, S. LEE, S.R. GARNER, J.C. ONG, S. KUEHN, J.A. MARÖHN, Dept of Chemistry, Cornell University — Magnetic resonance force microscopy (MRFM) is a technique that may one day allow us to acquire magnetic resonance images of single molecules. To date we have demonstrated that MRFM can achieve a sensitivity of ~10^8 proton spins, using a custom-fabricated silicon cantilever with a 9 micron diameter magnet tip. By making improved magnetic tips and mitigating surface dissipation, it may be possible to achieve single-proton sensitivity. Achieving the atom-scale force sensitivity necessary to image single proton spins requires custom-fabricating cantilevers with extreme dimensions. In MRFM the force exerted on the cantilever, per proton, is proportional to the field gradient from the cantilever's magnetic tip. Achieving single proton sensitivity requires a very small, densely packed array of magnet tips. We have developed an electron-beam-lithography (EBL) process for batch fabricating nanoscale tip magnets on ultrasensitive silicon cantilevers. Research by our group has shown that surface induced dissipation is a major source of noise, which can be minimized by fabricating the magnets overlapping the end of the cantilever. We will present 50-600 nm wide nickel overlapping magnets fabricated by EBL and isotropic plasma etching. With our designed cantilever, we expect a sensitivity of better than 10^7 protons.

K1.00109 Controlling and measuring substrate stiffness for cell motility studies, LINDSAY RUNYAN, PETER HOFFMANN, Wayne State University, KAREN BENINGO, Wayne State University — Cell motility and differentiation is generally considered to be controlled by an appropriate extracellular matrix (ECM). However, recent evidence has shown that mechanical cues may be just as important. Here, we present a study to create patterned substrates that allow us to test the hypothesis that cells prefer substrates of certain mechanical moduli and will migrate towards these substrates. In this context, we present a discussion of optimal methods to measure substrate moduli at the local level and compare different methods with respect to ease of implementation, data interpretation and reliability.

K1.00110 Measuring the energy landscape of complex bonds using AFM, ESSA MAYYAS, PETER HOFFMANN, LINDSAY RUNYAN, Wayne State University, HOFFMANN TEAM — We measured rupture force of a complex bond of two interacting proteins with atomic force microscopy. Proteins of interest were active and latent Matrix metalloproteinases (MMPs), type 2 and 9, and their tissue inhibitors TIMP1 and TIMP2. Measurements show that the rupture force depends on the pulling speed; it ranges from 30 pN to 150 pN at pulling speeds 300m/s to 48000m/s. Using timeresolved AFM, we studied the time evolution of the rupture force of studied MMP-TIMP interaction; we determined all physical parameters that form the landscape energy of the interaction, in addition to the life time of the bond and its length. Moreover, we used the pulling experiment to study the interaction of TIMP2 with the receptor MT1-MMP on the surface of living cells.

K1.00111 Scanning tunneling microscope-cathodoluminescence (STM-CL) imaging of the GaAs/AlGaAs (110) cross-section: evaluation of spatial resolution and imaging area shift, KENTARO WATANABE, Department of Applied Physics, School of Engineering, The University of Tokyo, YOSHIKI NAKAMURA, Quantum-Phase Electronics Center, Department of Applied Physics, School of Engineering, The University of Tokyo and CREST-JST, SHIGEYUKI KUBOYA, RYUJI KATAYAMA, KENTARO ONABE, Department of Advanced Materials Science, School of Frontier Sciences, The University of Tokyo, MASAKAZU ICHIKAWA, Quantum-Phase Electronics Center, School of Applied Physics, School of Engineering, The University of Tokyo and CREST-JST — We studied local optical properties of AlGaAs/GaAs multilayer structures by scanning tunneling microscope cathodoluminescence (STM-CL) spectroscopy, where low-energy (~100 eV) electrons field-emitted from STM tips were used as bright excitation sources. The STM-CL measurements were performed at the (110) cross-sectional surface of the AlGaAs/GaAs multilayer structure. We found that the field-emitted electron beam (FEEB) diameter mainly determine the spatial resolution of this system in STM-CL spectroscopy by evaluating some contributors: the thermalization length and the diffusion length of generated hot electrons. We also clarified that the shift of the STM-CL measurement position from the STM tip position was caused by the FEEB angled from the surface normal.

K1.00112 Twisted Pair Cryogenic Low Pass Filters, WOON SONG, Korea Research Institute of Standards and Science, MUSHTAQ REHMAN, SANG-WAN RYU, Chonnam National University, Korea, YOUNUK CHONG, Korea Research Institute of Standards and Science — For precise electronic-transport measurement at low temperatures, low pass filters are usually required to block external interference. However, since filters designed for the RF are not suitable for the field gradient from the cantilever's magnetic tip. Achieving single proton sensitivity requires a very small, densely packed array of magnet tips. We fabricated a low pass filter consisting of twisted pair of manganin wires wrapped in a copper tape, which can be made compact. We measured its microwave transmission characteristics with various filter parameters such as length, insulation thickness and twisted turns per unit length and compared the result with copper powder filter. The constructed filter with length of one meter showed a higher attenuation (more than 60 dB at 1 GHz) with cutoff frequency of about 8 MHz. This result is in good agreement with the theoretical model, which assumes the cable as a resistive transmission line.

K1.00113 Data Encoding on Continuous Wave THZ Signals for Sensing, KE SU, ZHIWEI LIU, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07102, LOTHAR MOLLER, Bell Laboratories, Alcatel-Lucent, Holmdel, NJ 07733, USA, JOHN F. FEDERICI, Department of Physics, New Jersey Institute of Technology, Newark, NJ 07032 — The intrinsic advantages of potentially ultra-high bandwidth, unrestricted frequency bands, and relative secure channels lead to a steadily increasing interest in THz communications. Other than for communication purposes, data modulation on THz signals could find application in sensing. When imprinting code sequences on pulse trains, ranging information from far distance scattering objects can be obtained to define selective measurement intervals. This technique is known from M-sequence radar and ultra-high bandwidth, multi-carrier modulation. A novel method of data encoding is described which combines these approaches with ultra-wideband, single-carrier modulation. The encoded signal is transmitted as a frequency modulated continuous wave (FM-CW) signal. The encoded data modulation is achieved by a digital phase modulation. An electro-optic phase modulator is used to directly modulate the THz wave through a τπ phase shift. While data rates in the MB/s range are demonstrated, it is possible to transmit data rates in the hundreds of MB/s range. Applications of the data modulation to sensing applications will be discussed.

K1.00114 Metal embedded Fiber Bragg Grating Sensors, CHOODA KHANAL, FIU, GARMAN VARGAS, KANTESH BALANI, ANUP KESHRI, CARMEN BARBOSA, ARVIND AGARIVAL, ROBERTO PANEPUCCI, FIU — A novel method of embedding optical fibers and optical fiber sensors, inside metallic structures will be discussed. We specifically report results for embedding fiber bragg grating sensors in an aluminum coating onto a steel plate. Characterization of an embedded FBG sensor and its effects on the sensor operation are also presented. Temperature sensitivity and the strain sensitivity will be discussed. The novel high throughput deposition method show the potential of embedding optical sensors onto metallic structures which make it suitable for many engineering applications in biomedical, civil, mechanical and aeronautical, among other fields.

K1.00115 Image contrast dependence on the field emitter in near field emission scanning electron microscopy, OLIVIER SCHOLDER, TARYL KIRK, LORENZO DE PIETRO, THOMAS BAELHER, URS RAMSPERGER, DANIELO PESCIA, Swiss Federal Institute of Technology Zurich (ETHZ) — In conventional scanning electron microscopy (SEM) the lateral resolution is limited by the electron beam diameter impinging on the specimen surface. Near field emission scanning electron microscopy (NFSEM) provides a simple means of overcoming this limit; however the most suitable field emitter remains to be determined. NFSEM has been used in this work to investigate the W (110) surface with single crystal tungsten tips of (310), (111), and (100)-orientations. The topographic images generated from both the electron intensity variations and the field emission current indicate higher resolution capabilities with decreasing tip work function than with polycrystalline W tips. Moreover the electron intensity images show more detail with higher resolution than field emission current imaging. This implies that the electron yield is more sensitive to additional parameters, which may be the local work function, specimen curvature, primary beam energy, and detector sensitivity.
Quantitative analysis of scattering force microscopy data using harmonic models

Thomas Henze, Klaus Schroeter, Albrecht Petzold, Thomas Thurn-Albrecht,
Institute of Physics, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — The separate identification of dissipative and elastic force contributions in Atomic Force Microscopy (AFM) is discussed. We show that within a harmonic approximation the interaction of the AFM tip with the sample surface can be described by average interaction parameters, namely an effective elastic tip-sample interaction $k_{eff}$ and an effective dissipation $\alpha_{eff}$, which can be extracted in a simple way from measured data. The method is applied to force spectroscopy curves on hard and soft polymeric model surfaces. The approach enables a thorough discussion of the influence of experimental parameters on the measured data. In imaging a clear identification of phases in systems with hard-soft contrast as for instance in semicrystalline polymers is made possible.

A nanoscopic study of degradation of optical recording media

Kwonjae Yoo, H.R. Kang, K.J. Kim, B.C. Woo, D.A. Ha, N.H. Lee, Wan S. Yun, KriSS, Daejeon 305-340, Korea, M.Y. Yun, Joongb University, Chungnam 312-702, Korea — The life expectancy of optical recording media usually depends on loss of physical property, that is, optical elements in digital recording unit cells eventually will be disappeared by physical and chemical degradation. Nevertheless, the study of information loss in the element by natural degradation is not so many, which need a practical and scientific investigation in detail. Here we present the results of the life expectancy estimation method of optical recording media studies on the recording unit cells by employing accelerated aging tool. Our results showed that archiving DVDs, which have double reflective layers, indicate the acceptable life expectancy over one hundred years. Additional optical, Surface Kelvin probe microscopy (SKPM) and electrostatic force microscopy (EFM) measurements clearly reveal the degradation of dye layer depending on accelerated aging time. The correlation between those physical quantities and PI errors might lead a key factor for the development of new life expectancy estimation method of optical recording media.

In-situ TEM observation on STM tunneling gap

Suhyun Kim, Yasumasu Tanishiro, Kunio Takayanagi, Tokyo Institute of Technology — Transmission Electron Microscope and Scanning Tunneling Microscope in an ultra high vacuum environment (UHV-TEM-STM) have been combined to simultaneously perform both high resolution TEM and atomically resolved STM experiments. This system was constructed for in-situ investigation of physical property of impurity atoms embedded below semiconductor surface. To image TEM and STM at the same time, crucial requirement is that, the STM image must be acquired under the electron beam irradiation. As a preliminary test, we used HOPG (Highly Oriented Pyrolytic Graphite) sample and tungsten tip as schematically shown in Fig 1(a). Fig 1(b) shows an atomic resolution STM image of HOPG obtained with 300mV sample bias and 3nA tunneling current even in the condition of the electron beam irradiation on the tip. TEM image can be simultaneously acquired by performing In-situ TEM observation on STM tunneling gap formed between the tip and a thin sample. Fig 1(a) Geometry of STM observation on STM tunneling gap Fig 1(b) STM image of HOPG obtained with 300mV sample bias and 3nA tunneling current

Micromechanical devices for magnetization measurements at high magnetic fields and low temperatures

J. Paster, K. Ninios, H.B. Chan, University of Florida, L. Balicas, Florida State University — We constructed micromechanical faraday balance magnetometers for measuring the absolute value of the magnetization of very small samples (~ 1ugram) at high magnetic fields and a wide range of temperatures. The magnetometers consist of a movable polycrystal silicon plate (500 by 500 micrometers) suspended by four springs above a fixed electrode. When small samples of the magnetic material are placed at the center of the movable plate, the magnetic field gradient creates a force on the sample that changes the capacitance between the plate and electrode. The absolute magnetization of the sample can be determined provided that the magnetic field gradient is known. Springs with different shapes are designed to minimize the response to magnetic torque. Experimental results will be compared to numerical simulation.

X-ray Young’s double slit experiment and other aspects of kinoform X-ray prism arrays

A.F. Isakovic, K. Evans-Lutterodt, BNL-NSLS, A. Stein, J.B. Warren, BNL-CFN, S. Narayanan, A.R. Sandy, ANL-APS — Numerical design and large aspect ratio nanofabrication techniques [1] were employed to produce kinoform prisms and lenses for the purpose of focusing, deflecting and characterizing hard X-ray synchrotron radiation. Purely refractive prisms are hampered by the effects of absorption, which limits the numerical aperture of the lens and hence the optic resolution. Kinoform lenses allow one to circumvent these limitations, with the trade-off of an energy bandwidth for the optic. Purely refractive prisms have similar limitations due to absorption, and consequently we choose to fabricate kinoform prisms and study their properties experimentally. In particular we analyze theoretically the extent to which the kinoform prism can be modeled by a simple prism, and the effect of nano-fabrication precision on the prism performance. The focus of the nano-fabrication efforts is in balancing out patterning of a large area and a deep anisotropic etch. Experimental characterization is performed at APS 8-ID beamline. We observed, controlled and measured interference fringes, in analogy with the Young’s double slit experiment. [1] A. F. Isakovic et al., JVST-A 26, 1182 (2008) and J. Synchr. Rad. 16.
Characterization of the Throughput of Short Fiber-Optic Arrays as a Function of the Angle of Incidence

An instrument was constructed to measure the light distribution at the back of a thin fiber-optic array as a function of the angle of incidence and the location at which the incoming 633 nm light strikes a fiber. The f-number of the incoming light is 10 and the diameter of the focal spot is 8 microns. The input optics are mounted on a rail that rotates in such a manner that the focal location remains fixed. Images of the light distribution at the back of the array are recorded using a 12-bit 2.5 megapixel camera. Data recorded using commercial face plates is presented.

Nano-scale Spin State in Invar Alloy Fe-36at%Ni

PENG ZHAO, P. CHRIS HAMMEL, Department of Physics, Ohio State University, JI-CHENG ZHAO, Department of Material Science and Engineering, Ohio State University — We use high-resolution ferromagnetic resonance force microscopy (FMRFM) to image the nano-scale spin structure of an Invar alloy (Fe-36at%Ni) to test the well-known two-spin-state hypothesis proposed by Weiss. Weiss proposed that the two-spin-state model could explain the Invar effect; but to our knowledge this has not been experimentally confirmed. With nano-scale spatial resolution of FMRFM, we intend to experimentally examine the existence or absence of such states in the Fe-36at%Ni Invar alloy.

Chemical Physics

Salt-induced overcharging, charge inversion and reentrant condensation in polyelectrolyte solutions

The behavior of highly-charged polyelectrolytes (PE) in multivalent salt solutions is investigated by computer simulations. By studying the charge distribution function around a chain, we show that PE is charge-overcompensated near its surface by condensed multivalent counterions when salt concentration is high. Nonetheless, the effective chain charge, computed by the ratio of the electrophoretic mobility to the diffusive mobility, can be positive or negative, depending sensitively on the ion size. This finding violates our intuitive thinking that an overcharging on the surface of a charged macromolecule leads inevitably the sign inversion of its effective charge. Moreover, the reentrant condensation of PE is studied by calculating the mean distance between chains. Chain aggregation happens only when salt concentration is intermediate and the ion size is comparable to the monomer size. The results demonstrate the importance of ion excluded volume and suggest a disconnection of the salt-induced segregation of PE chains at high salt concentrations with charge inversion.

Free energy landscapes of short polyproline peptides in vacuo and solvated environments

MAHMOUD MORADI, CHRISTOPHER ROLAND, VOLODYMYR BABIN, CELESTE SAGUI, CHIPS and Department of Physics, North Carolina State University — Polyproline peptides are known to occur in two different conformations, including right-handed PPI and left-handed PPII. Depending on the solvated environment and the peptide length, either PPI or PPII is favored. Specifically, we calculated the free energy landscapes of short polyproline peptides (length 6, 9, 13-mers) in vacuo, in implicit water, and in the solvents hexane and propanol as a function of the radius of gyration and handedness. To calculate the free energies, the recently developed Adaptively Biased Molecular Dynamics (ABMD) method, which belongs to the general category of umbrella sampling methods with a time-dependent potential, was used.

In situ sum-frequency generation spectroscopy of ethylene-glycol and poly-N-isopropylacrylamide films

VOLKER KURZ, PATRICK KOELSCH, University Heidelberg — Ethylene-glycol(EG)-based self-assembled monolayers (SAMs) are often used as a model systems for thin liquid films. Temperature series in heavy water were measured using a unique sample cell developed for in situ sum-frequency generation (SFG) spectroscopy experiments. Results obtained from model EG-SAMs with different lengths and terminations groups in various ion solutions showed temperature-dependent changes in the molecular order. Films of poly-N-isopropylacrylamide(pNIPAM) were also characterized by in situ SFG spectroscopy in the CH, OH, OD and amide spectral regions under different polarization combinations. These systems have many applications as thermo-responsive polymers due to their ability to change solubility in water at the biologically relevant temperature of 32 °C. This so-called lower critical solution temperature (LCST) phase transition was characterized in depth, allowing for the identification of the molecular groups involved in this process.

The Effects of Multiwalled Carbon Nanotube Doped Poly(Ethyl Methacrylate) on Optical Field Induced Nematic Liquid Crystal Reorientation

MATTHEW KERR, DAVID STATMAN, Allegheny College — We have been investigating photoinduced gliding of the easy axis at the nematic liquid crystal/polymer interface. Gliding of the easy axis on polyethylene methylacrylate (PEMA) surfaces has been observed when magnetic or electric fields are applied to the bulk liquid crystal. We have studied similar gliding when the surface is coated with a carbon nanotube/PHEMA composite. Our experiments utilize polarimetry techniques and cross-polarized microscopy. The results of photoinduced gliding experiments on PEMA surfaces doped with multiwalled carbon nanotubes will be presented.

Mapping hydration dynamics and coupled water-protein fluctuations around a protein surface

LUYUAN ZHANG, LIUJAN WANG, YA-TING KAO, WEIHONG QIU, YI YANG, OGHAGHARE OKOBIAH, DONGPING ZHONG, The Ohio State University — The behavior of highly-charged polyelectrolyte solutions is investigated by computer simulations. By studying the charge distribution function around a chain, we show that PE is charge-overcompensated near its surface by condensed multivalent counterions when salt concentration is high. Nonetheless, the effective chain charge, computed by the ratio of the electrophoretic mobility to the diffusive mobility, can be positive or negative, depending sensitively on the ion size. This finding violates our intuitive thinking that an overcharging on the surface of a charged macromolecule leads inevitably the sign inversion of its effective charge. Moreover, the reentrant condensation of PE is studied by calculating the mean distance between chains. Chain aggregation happens only when salt concentration is intermediate and the ion size is comparable to the monomer size. The results demonstrate the importance of ion excluded volume and suggest a disconnection of the salt-induced segregation of PE chains at high salt concentrations with charge inversion.

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K.00132 Quantized ionic conductance in nanopores, MICHAEL ZWOLAK, Los Alamos National Laboratory, JOHAN LAGERQVIST, MASSIMILIANO DI VENTRA, University of California - San Diego — We study ion transport through nanopores via molecular dynamics calculations. Due to the confined geometry and large local field of a single ion, the nanoscale atomic configurations of species influence the ionic conductance. In particular, hydration layers that form around ions in aqueous solution create a series of energy barriers to ion transport. As an ion enters the pore, these hydration layers have to be partially broken due to steric restrictions of the pore. The breaking of the layers proceeds in a highly nonlinear, step-like fashion, giving rise to a strong nonlinear dependence of the electrostatic energy barrier on the pore diameter and therefore also a step-like conductance. We discuss this effect as well as the conditions under which it may be experimentally observed. 1

1This work has been supported by NIH and Los Alamos

K.00133 Base sequence dependence and backbone-induced effects on charge transport through DNA, YONG JOE, SUN LEE, ERIC HEDIN, Ball State University — We investigate quantum mechanical electron transmission along the long axis of the DNA molecule using a tight-binding model. Specifically, we use two different DNA models to study the charge transfer efficiency of synthetic ds-DNA. First, the generic form of a simple one-conduction channel model, called the fishbone model, is used. The sugar-phosphate backbone and the coupling amplitude between each site of the base and the backbone are incorporated into an energy-dependent on-site potential in the main DNA site. Here, individual sites represent a base-pair formed by either AT (TA) or GC (CG) pairs coupled via hydrogen bonds. Second, we employ a two-dimensional three-chain model where the backbone on-site energy, the coupling amplitude between the bases and the backbone, and a possible hopping of charge carriers between the successive backbone sites are used as key parameters. The overall transmission and the current-voltage characteristics are calculated to determine the influence of mismatch (impropriety) effects in the DNA sequence. Finally, we discuss the transmission gap as a function of coupling between the bases and between the bases and the backbone. *One of the authors (E.R.H) is partially supported by a grant from the Center for Energy Research, Education, and Service (CERES) at Ball State University.

K.00134 Lanthanide Metal-Organic Framework Materials, PING-YEN HSIEH, University of Maryland-College Park, MARK A. GREEN, National Institute of Standards and Technology, ROBERT M. BRIBER, University of Maryland-College Park — A series of lanthanide metal-organic framework materials (MOF) with variable organic linkages including benzene-dicarboxylic acid (BDC), 1,3,5-benzene-tricarboxylic acid (BTC), and 1,3,5-tris(4-carboxyphenyl)benzene (BTB) have been synthesized. The low density and high porosity of MOFs make them candidates molecular sieve or hydrogen storage materials. The crystal structures have been determined using a combination of single crystal X-ray diffractometer and synchrotron powder X-ray diffraction work. Holmium with the BDC ligand material (Ho-BDC) crystallizes in a monoclinic C2/c space group, with lattice parameters of a = 17.06 Å, b = 10.67 Å, c = 10.57 Å, β = 96.12°. The crystal structure of Ho-BTC is in tetragonal P 41 2 2 space group and Ho-BTB is in a triclinic P-1 space group. A comprehensive examination of Ho-MOF with different ligands by x-ray and thermogravimetric analysis shows that there is a stable nanoporous structure for dehydrated Ho-BTC up to 250°C. The same phenomenon is not observed in the Ho-BDC and Ho-BTB materials. The collapsed structure with BDC and BTB indicates the stability of dehydrated samples is strongly related to the interactions between the metal and the organic linkers.

K.00135 Ultrafast Spectroscopy of Single-Stranded Adenine Oligomers, CHARLENE SU, The Ohio State University, CHRIS MIDDLETON, University of Wisconsin-Madison, BERN KOHLER, The Ohio State University — The excited-state dynamics of single-stranded homo-oligomers containing a variable number of adenine bases have been studied by femtosecond transient absorption technique within the ground state absorption band. The bleach recovery signals show that all the adenine oligomers decay with a long-lived component of a hundred picosecond in addition to a short-lived component, which is also observed in the adenine mononucleotide, 2'-deoxyadenosine 5'-monophosphate. The latter component is attributed to vibrationally cooling to the electronic ground state and the former one is associated with intrastrand excimer formation between stacking bases. It is found that the amplitude of long-lived component increases with the elongation the of adenine oligomers in comparison to the short-lived one. Excimer yields estimated on the basis of relative amplitude show that adenine oligomers have higher excimer formation in longer strands, indicating a greater degree of base stacking.

K.00136 Homogeneous bubble nucleation in liquids: a molecular dynamics study, ZUN-JING WANG, Carnegie Mellon University, CHANTAL VALERIANI, University of Edinburgh, DAAN FRENKEL, University of Cambridge — We have studied homogenous bubble nucleation in a Lennard-Jones fluid by performing Molecular Dynamics simulation coupled with Forward-Flux Sampling (MD-FFS). The MD-FFS estimate of bubble-nucleation rate is higher than predicted on the basis of Classical Nucleation Theory (CNT). Although this discrepancy is consistent with earlier findings, our simulations show that bubble nuclei are compact rather than ramified as had been suggested by Shen and Debenedetti (J. Chem. Phys. 1999, 111:3581). We find bubble nucleation starts with local spots much hotter than superheated environment, and the local temperature correlates strongly with subsequent bubble formation - this mechanism is not taken into account in CNT.

K.00137 Investigation into the Mpemba Effect: Variation in the Freezing Time of Water Dependent on Initial Temperature and Purity, INGRID THVEDT, MARTHA ROSEBERRY, SUSAN LEHMAN, The College of Wooster — The observation that hot water sometimes appears to freeze more quickly than cold water, known as the Mpemba effect, has generated vigorous debate. Prior research [1] into the Mpemba effect has resulted in conflicting results, due to a variety of observation techniques, multiple definitions of freezing, and different water treatments. To clarify the previous results, we have tested multiple types of water and improved the sample monitoring. During cooling and freezing, each 50 g water sample is continually monitored by three thermistors at different depths. Samples of tap, distilled, and nanopure water were heated, heated and cooled, or boiled before being frozen. We monitor the time to reach freezing, the duration of freezing, and the total time to reach -7°C. We observe the Mpemba effect most consistently in the length of the freezing transition in tap water. Observations of temperature variation during freezing will also be presented. [1] See the review by M. Jeng, Am.J.Phys. 74 S14 (2006).

This research was supported by NSF-DMR 0649112 and The College of Wooster.

K.00138 Clockwork Rotation and Rotation Transduction in 2D crystals of Janus amphiphilic colloidal spheres, SHAN JIANG, STEPHEN ANTHONY, STEVE GRANICK, University of Illinois at Urbana and Champaign — Colloidal spheres with one side hydrophilic and the other side hydrophobic can self-assemble into clusters owing to amphiphilicity. When the particle concentration is high enough, 2D crystals with hexagonal translational order and additional orientational order will form. By using the Fourier Transform and particle tracking techniques, the position and the rotation of each single particle can be tracked. Long-range clockwork rotation behaviors were observed for the particles inside the clusters. In other words, when one particle rotates by Brownian motion, the particle next to it is impelled to counter-rotate. This transduction extends for a distance up to half a dozen particles.
K.100139 Modeling Chemical Reactions on Metal Oxide Surfaces, HAITAO LIU, University of Pittsburgh, MICHAEL FALCETTA, Grove City College, KENNETH JORDAN, University of Pittsburgh — Photocatalytic conversion of carbon dioxide to methanol has been observed at titanium dioxide interfaces, but the detailed mechanisms are unknown. Computer simulations can prove valuable in elucidating the mechanisms and aid in improving the efficiency. Two major computational strategies for treating such systems are slab and cluster models. The present work uses both periodic slab and embedded cluster models to elucidate the important factors in developing an embedding scheme that properly treats the system and allows the treatment of excited electronic states. Ground state adsorption energies are calculated for a variety of basis sets, cluster sizes, electronic structure methods and embedding schemes to demonstrate convergence with respect to all of these variables. Detailed comparisons of the electrostatic potential obtained from periodic and embedded cluster models are presented to clarify the importance of various effects in the embedding scheme.

1Supported by National Science Foundation and National Energy Technology Laboratory.

K.100140 Spontaneous spreading of particle monolayers from unstable Pickering emulsions, HSIN-LING CHENG, SACHIN VELANKAR, Chemical Engineering, University of Pittsburgh — Partially-wettable particles can adsorb at liquid/liquid interfaces and give stable Pickering emulsions. However, if there are insufficient particles, then the emulsion is unstable. In such an unstable emulsion, we document a remarkable phenomenon, viz. coalescence of an oil/water/particle Pickering emulsion contained in a vial induces a particle film to climb up the walls of the vial. While this has been noted previously with nanoparticles, we show that such film-climbing is highly general and can be induced by a variety of particle types, particle sizes ranging from a few nm to a few microns, and different emulsion types. Many of the features of film growth described previously with nm-sized particles are found to remain true even with the far larger particles studied here. Binks et al., Langmuir, 22, 4100, 2006, have postulated that the particle films that climb up the walls of a vial are actually comprised of one oil layer and one water layer, with particles adsorbed at the interface between them. We confirmed this “sandwich” structure experimentally and also show that such interfacially-adsorbed particles can easily exert the very modest surface pressure necessary to sustain the weight of the film. Finally, while some climbing films are tightly-packed particle monolayers, tight packing is not essential; even sparsely-populated monolayers can display film climbing.

K.100141 Kinetics and Cross-Stream Migration of Polymer Solutions in Nanoscale Channel Undergoing Shear Flow, JAIME A. MILLAN, SIDY DANIOKO, MOHAMED LARADJI, University of Memphis — Polymer solutions confined to nanoscale slit pores are investigated in detail via generalized dissipative particle dynamics. We focus both on Poiseuille and planar Couette flows. In both cases, we investigated the effect of Schmidt number through the modification of both random and dissipative forces. The trend of the cross-stream migration of the polymer chains depends strongly on the value Schmidt number of the solution. In particular, we found a migration towards the walls for relatively low Schmidt number. However, polymer migration toward the channel centerline is observed for relatively high Schmidt number, in agreement with experimental observations and simulations based on other numerical approaches. The polymer chains kinetics is characterized by tumbling with well-defined characteristic time scale that decreases with increasing shear rate. The power spectra of both polymer stretch and tilt are in agreement with recent experiments.

1Supported by the Petroleum Research Fund.

K.100142 Synthesis, characterization and optical properties of magnesium hydroxide micro-/nanostructures, LATHA KUMARI, WENZHI LI, Florida International University, CHARLES H. VANNOY, ROGER M. LEBLANC, University of Miami, DEZHI WANG, Boston College, DEPARTMENT OF PHYSICS, FLORIDA INTERNATIONAL UNIVERSITY, MIAMI, FL 33199, USA TEAM, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MIAMI, CORAL GABLES, FL 33124, USA COLLABORATION, DEPARTMENT OF PHYSICS, BOSTON COLLEGE, CHESTNUT HILL, MA 02467, USA COLLABORATION — Magnesium hydroxide (Mg(OH)2) crystals of various shapes and sizes (micron to nano) were synthesized by single step hydrothermal route at different reaction conditions. The as-prepared hexagonal (Mg(OH)2) particles were converted to cubic MgO by calcination at 450°C. The Mg(OH)2 and MgO nanostructures showed optical band gaps of 5.7 and 3.43 eV, respectively. Broad band photoluminescence emission spectra were observed in the vicinity of UV and visible region. Mg(OH)2 and MgO nanostructures with wide optical band gap and short-wavelength luminescence emission can be used as a luminescent material for photonic applications.

1W.Z. Li acknowledges the support by National Science Foundation under grant DMR-0548061.

K.100143 Fabrication of zinc oxide microstructures and their properties, LATHA KUMARI, WENZHI LI, Florida International University, CHARLES H. VANNOY, ROGER M. LEBLANC, University of Miami, DEZHI WANG, Boston College, DEPARTMENT OF PHYSICS, FLORIDA INTERNATIONAL UNIVERSITY, MIAMI, FL 33199, USA TEAM, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MIAMI, CORAL GABLES, FL 33124, USA COLLABORATION, DEPARTMENT OF PHYSICS, BOSTON COLLEGE, CHESTNUT HILL, MA 02467, USA COLLABORATION — The bitter-melon-like and prism-like zinc oxide (ZnO) microstructures have been synthesized by hydrothermal route. Besides these microstructures, the ZnO material also consists of spherical nanoparticles with narrow size distribution. The as-synthesized ZnO material depicts hexagonal crystal structure. An optical band gap of 2.95 eV is determined from the UV-vis absorption band edge. The prism-like ZnO microstructure shows an ultraviolet near-band-edge emission at about 3.27 eV (380 nm) at room temperature which can be assigned to the radiative annihilation of excitons. The wide-band gap oxide materials like ZnO with short-wavelength PL emission can find application in light emitting devices.

1W.Z. Li acknowledges the support by National Science Foundation under grant DMR-0548061.

K.100144 Size dependent thermalization time of Ag nanoparticles and the surface density profile, CATALINA LOPEZ-BASTIDAS, Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autonoma de Mexico, Ensenada, Baja California, Mexico — It is well known that the lack of d-electron screening in the s-electron spill-out region at the surface of Ag nanoparticles increases the electron-electron interaction in this region compared to the bulk. Therefore when comparing the electron-electron interaction contribution to the thermalization time of Ag nanoparticles of varying radius, smaller particles thermalize faster due to the increased surface to bulk ratio. One aspect which has not been addressed is the effect of the spatial distribution of charge at the surface of the nanoparticle. In this work it is shown that the size dependence of the thermalization time is very sensitive to the surface density profile. The electron thermalization time of conduction electrons in Ag nanoparticles as a function of the radius is calculated. The sensitivity of the scattering rate to the spatial distribution of charge at the surface of the nanostructure is analyzed using several model surface profiles. The change in surface charge distribution via charging or coating of the nanospheres is shown to be a tool for control and probing of the ultra-fast electron-electron dynamics in metallic nanoparticles.
K1.00145 A General Route to Inorganic Nanoparticles Using a Condensed Electron Beam, MARISSA CALDWELL, Stanford University, SHAUL ALONI, JEFFREY URBAN, DELIA MILLIRON, LBLN, H.-S. PHILIP WONG, Stanford University — Inorganic nanoparticles are of interest to study the size dependence of various material properties. However, current colloidal synthetic routes are limited in the scope of accessible inorganic materials. Here we present a facile route to inorganic nanoparticles of a wide range of material compositions and sizes. Using the beam from an electron microscope, 2 – 100nm particles were formed from micron sized pieces of a wide range of materials including: semiconductors, metals, insulators. Using this route, we have produced nanoparticles of over 25 different compositions. Each material demonstrated an energetic threshold barrier to particle formation. To help elucidate the formation mechanism, we collected cathodoluminescence spectra which, when correlated with known temperature-dependent bandgap data, showed a large increase in temperature due to the e-beam-to-material interaction. The temperature rise dependence on the e-beam current and acceleration voltage was studied. We conclude that the temperature rise is large enough to compare with vaporization energies and is a plausible mechanism for the production of nanocrystals.

K1.00146 Can isolated Au nanoclusters catalyze CO oxidation?, P.-S. LIN, A.-L. CHIN, C.-P. CHANG, F.-K. MEN, Department of Physics, National Chung Cheng University, Chia-Yi, Taiwan, R.O.C. — It has been more than twenty years since the discovery of oxide-layer supported Au nanoclusters (<5 nm) capable of catalyzing CO oxidation. This discovery has attracted a lot of attention owing to possible practical applications as well as a model system for understanding nanoscale catalysis. One mechanism that has been proposed to explain this observation is that the process takes place entirely on Au nanoclusters. Since most experiments performed on this topic have been done in complicated environments, it would be difficult to fully justify/dismiss the validity of a particular mechanism. We have chosen a clean and inert support, highly oriented pyrolytic graphite, to grow Au nanoclusters via molecular beam epitaxy under ultrahigh vacuum conditions. We measured the change in CO$_2$ partial pressure after leaking high-purity CO and O$_2$ gases into the vacuum chamber with and without the presence of Au nanoclusters. To perform a systematic investigation, we also prepared Au nanoclusters of different densities and sizes. With the presence of Au nanoclusters we could not find any discernible increase in the CO$_2$ partial pressure, thus rules out the possibility that Au nanoclusters would take a full credit in catalyzing CO oxidation.

K1.00147 Chemical Synthesis and Characterization of Self-Assembled Nanoparticles Prepared in the Presence of Citrate Ions, KARL UNRUH, THOMAS EKIERT, University of Delaware — Iron(II) ions in aqueous solutions containing various concentrations of citrate ions have been reduced to metallic Fe using sodium borohydride. In comparison to the 10-20 nm diameter Fe particles formed in the absence of citrate, the presence of citrate results in the formation of 100–200 nm spherical (or in some cases cubical) particles self-assembled from much smaller Fe nanoparticles. Structural, chemical, and magnetic measurements indicate that for appropriate citrate/Fe ratios, air stable powders that exhibit a room temperature saturation magnetization of nearly 200 emu/g and a coercivity less than 100 Oe – even without deoxygenating the reaction solution or an explicit surface passivation step – can be obtained. Thermal treatments at temperatures between 350 and 450 °C result in the sintering of the Fe nanoparticles within the larger aggregates while heat treatments at higher temperatures result in the sintering of the aggregates themselves into a continuous porous matrix.

K1.00148 Brownian Motion of an Ellipsoid in Correlated Fluids, SHAOQING ZHANG, University of Pennsylvania, WU-PEI SU, University of Houston — To account for the correlation in the fluctuation force due to the surrounding media, we analytically study the diffusive behavior of an anisotropic Brownian particle by introducing an exponentially correlated colored noise in the rotational motion. The crossover from anisotropic to isotropic diffusion slows down, and the increase in the translational diffusion coefficient induced by an external force is enhanced. These results are of great interest in the research on biological physics and soft matters.

K1.00149 Enantiospecific Interaction of Histidine with Planes of Single Crystalline alpha Quartz, DANISH FARUQUI, PAUL J. SIDES, VLADIMIR V. PUSHKAREV, ANDREW J. GELLMAN, Carnegie Mellon Univ — Chiral chemistry profoundly affects living organisms because they are homochiral environments. The origin of life itself trace to enantiospecific interactions. Chiral purity is an important scientific and technological goal. Adsorption of chiral compounds on ‘powdered’ quartz is sometimes enantioselective. Here we offer positive evidence of diastereomeric, chiral recognition at the interface between ‘single crystal’ alpha quartz and aqueous histidine and verification of the effect for three principal crystallographic orientations of quartz. Characterizing the electrostatic environment, the zeta potential of (0001) L-quartz decreased by approximately 40 mV±5 as R-histidine was added incrementally to a concentration of 400 u molar; the zeta potential of the same L-quartz sample, however, decreased by only 20 mV±5 in an otherwise identical experiment with L-histidine. Results of all diasteriomeric and control experiments on each plane were consistent, the zeta-potential provides evidence that adsorption on quartz is enantiospecific; is influenced by the chirality of quartz but not necessarily by the crystallographic orientation of the surface.

K1.00150 Electronic Structure of Ti substituted hydroxypatite: TiHap, SHUXIA YIN, DONALD ELLIS, Northwestern University — Hydroxyapatite (Hap), with the chemical formula Ca$_{10}$(PO$_4$)$_6$(OH)$_2$, is the main mineral constituent of mammal tooth enamel and bone and has become an important biomaterial with medical applications. Hap also attracts increasing interest for use in environmental adsorbents and catalysts due to its porous nature and highly active ion-exchange character. Ti-modified Hap (TiHap) has been proved to possess high affinity to organic molecules and bacteria as well as high photocatalytic activity for their oxidative decomposition. The concentration of Ti$^{4+}$ is a key factor controlling TiHap crystallinity and catalytic efficiency. Here we studied the sorption mechanism of Ti$^{4+}$ on Hap using Density Functional Theory within periodic slab models. Ti$^{4+}$ or (Ti(OH)$_2$)$^{2+}$, as the most likely ion exchange species with Ca$^{2+}$, were first considered in bulk Hap. A second charge compensated model considered includes both surface Ca ion vacancies and substitutional Ti$^{4+}$. To obtain insight of the energetic stability and microscopic crystal structure of TiHap, Ti substitution on different Ca sites and distributions at different atomic ratios are investigated in both bulk and surface models.

1 Supported by US DOE, at Northwestern Institute for Catalysis in Energy Processes.
K1.00151 Time-Dependent Density Functional Theory Applied for Pulse Laser Shot: Criterion of the Numerical Stability1. YOSHIYUKI MIYAMOTO, CREST-JST, Nano Electronics Res. Labs. NEC, HONG ZHANG, Sichuan University — In this talk, applications of TDDFT [1] for irradiation of pulse laser to materials and subsequent structural change are shown. Contrary to the pioneering works [2-3], we present a way of judging numerical stability which can be confirmed by the energy conservation rule. The conserved quantity is the DFT total energy plus kinetic energy of ions minus work done by the pulse shot [4], which can simply be demonstrated with use of adiabatic exchange-correlation functional and time-varying electric field generated by a time-varying fictitious charge. As an example, structural change on graphite surface induced by pulse laser shot is demonstrated with use of 10-layer AB-stacked slab model. After irradiating laser shot with wavelength of 800 nm, pulse width of 50 fs, and a power about 90 mJ/cm² per pulse, the top graphene monolayer spontaneously leaves while other layers remain.


1All calculations were performed by using the Earth Simulator.

K1.00152 Enhanced Surface Plasmon Resonance. WEIQIANG MU, Northwestern University, JOON JANG, Northwestern University, MAXIM SUKHAREV, Arizona State University, DONALD BUCHHOLZ, ROBERT CHANG, JOHN KETTerson, Northwestern University, KETTERSON TEAM, CHANG TEAM, SUKHAREV TEAM — We have studied the surface plasmon resonances in thin silver films sandwiched between silica. This is the so-called Sarid geometry which supports a (short-range) symmetric and a (long-range) anti-symmetric mode. The coupling is achieved diffusively via an approximately sinusoidal surface etched in the underlying silica prior to deposition of a 20nm Ag film and a 400nm silica capping layer; the modulation amplitudes were 10, 30 and 50nm. FDTD simulations of the transmission (T) and reflection (R) coefficients show that for perpendicular incidence strong coupling occurs to the two plasmon modes along with a much weaker electromagnetic Woods anomaly. We will present data on both T and R showing evidence of coupling to the antisymmetric and symmetric Sarid modes as well as observations of waveguiding effects in the silica capping layer. Data will be compared with FDTD calculations for corresponding film parameters.

K1.00153 Changing What Science Is and How It’s Done. ROBERT JONES — Knowledge is of an approximate character. Our formalisms abstract and simplify. Each formalism is an idealization, often times approximating in its own DIFFERENT ways, each offering somewhat different coverage of the domain. Having MULTIPLE overlapping theories of a knowledge domain is then better than having just one theory (R. Jones, APS Gen. Meeting, March 2008 and refs. therein). In the future each field will possess multiple theories of its domain and scientific work and engineering will be performed based on the ensemble predictions of ALL of these. This idea can be considered an extension of Bohr’s notion of complementarity, “...different experimental arrangements...described by different physical concepts...together and only together exhaust the definable information we can obtain about the object.” Although finding the “correct” or “most probable” theory has been the goal of scientific investigation in the past we now know that the pluralistic science that I am describing here is more successful (Peter Cheeseman in The Mathematics of Generalization, D. H. Wolpert, Ed, 1995, pg. 315 and Michael Weisberg, J. of Philosophy, 2007, pg. 646). This is not postmodernism. Theories are accepted based upon experimental evidence not human opinion. Over the years I have tried to keep with this new pluralism in both my fusion energy and artificial intelligence work.

K1.00154 The Role of the Element Rhodium in the hyperbolic law of the Periodic Table of Elements. ALBERT KHAZAN — The method of equilateral hyperboles assumes that their tops should be certain with high accuracy by means of Lagrange’s theorem. On this basis the scaling factor for transition from the coordinate system usual to mathematicians to that which is to be used in chemistry is calculated. Such an approach has allowed calculating parameters of the last element. The calculation can be checked by means of the first sequel from the hyperbolic law, proceeding only from the atomic mass of the element Rhodium. As it has appeared, the direct and adjacent hyperboles are crossed in a point with the coordinates 205.811; 0.5, which abscissa makes a half of the last element’s atomic mass (the deviation is about 0.01%). The real axes of the hyperboles coincide with the tangents and normals, and the scaling factor differs from the first calculation as 0.001%. However these insignificant divergences are so small to the most important conclusion that the validity of the Hyperbolic Law, as calculation on Rhodium our data consists of (Progr. Physics, 2007, v.1, 38; v.2, 83; v.2, 104; 2008, v.3, 56).

K1.00155 Coordination of Swarmed Unmanned Ground Vehicles using Self Organization Mapping with Generic Algorithm1. SHEKHAR PRADHAN, DeVry College of New York — The methodologies for path planning for individual UGVs have been well studied and modeled. The Simultaneous Localization and Mapping (SLAM) is an example of such study. However, there is no reliable method of communication among swarmed UGVs. The author along with other collaborators, Dr. Wei Cao of NASA Research Center and Dr. James Burghart of Cleveland State University, proposes a Master-slave approach for the coordinated management of UGVs using Neural Networks. SOM is used to work with the coordinates 205.811, 0.5, which abscissa makes a half of the last element’s atomic mass (the deviation is about 0.01%). The real axes of the hyperboles coincide with the tangents and normals, and the scaling factor differs from the first calculation as 0.001%. However these insignificant divergences are so small to the most important conclusion that the validity of the Hyperbolic Law, as calculation on Rhodium our data consists of (Progr. Physics, 2007, v.1, 38; v.2, 83; v.2, 104; 2008, v.3, 56).

1The research is supported by NAVY and NASA grants.

K1.00156 Effects of Aggregation on the Electronic Properties of Polyyiophene and its Oligomers. KELLY ZEWE, LINDA PETEANU, WYNEE LEE — Polyyiophene is a commonly used component of organic electronics and solar cells. Polyyiophene chains are readily aggregated under the processing conditions used to form thin films for applications in devices. This aggregation can drastically alter the charge transfer and optical properties of the material. In order to better understand these effects, oligomers of polyyiophene were studied. Because oligomers have shorter, well-defined chain lengths and are free of defects, the effects of aggregation on their electronic properties are easier to interpret than those of the polymer systems and are more readily modeled using electronic structure theory. Bulk and single-molecule fluorescence methods are used to explore the emission properties as a function of aggregate size, precipitating solvent, and monomer properties and to correlate these to the polymer properties. Stark spectroscopy is used to measure the change in charge separation and in excited-state delocalization caused by aggregation and the consequent increase in chain-chain contacts.
K1.00157 Adsorption on Nanotubes With Repulsive First Neighbors\textsuperscript{1}. ALAIN PHARES, Villanova University, DAVID GRUMBINE, St. Vincent College, FRANCIS WUNDERLICH, Villanova University — We consider adsorption on nanotube lattices with zigzag triangular geometry. In Langmuir, Vol. 24, pp. 11722-11727 (2008), we studied such adsorptions with first- and second-neighbor interactions and attractive first-neighbors. The nanotube energy phase diagram is independent of \( M \), the number of atoms in the nanotube circumference, and holds for infinite \( M \), reproducing the infinite width limit of a triangular terrace [Langmuir, Vol. 24, pp. 124-134 (2008)]. Here, we consider repulsive first-neighbors. The phase characteristics, \( \{\theta_0, \theta, \beta\} \), are the coverage, and the numbers per site of first and second neighbors, respectively. Particle-hole symmetry holds for all nanotube diameters and the energy phase diagram is \( M \) dependent. In the infinite-\( M \) limit, the non-trivial phases with their complements are: \( \{1/4, 0, 0\} \), or \( \{2 \times 2\} \), and \( \{3/4, 3/2, 3/2\} \); \( \{1/3, 1/3, 0\} \), or \( \{3 \times 1\} \), and \( \{2/3, 4/3, 1\} \); \( \{1/3, 0, 1\} \), or \( \{\sqrt{3} \times \sqrt{3}\} \); \( \{2/3, 1, 2\} \); and \( \{1/2, 1/2, 1/2\} \), which is its own complement. This infinite-\( M \) limit should be the same as the infinite width limit of a triangular terrace. We found that we had missed the \( \{2/3, 4/3, 1\} \)-phase in Langmuir, Vol. 23, pp. 1928-1936 (2007).

\textsuperscript{1}Work supported by NSF and the Pittsburgh Supercomputing Center.

K1.00158 Fast algorithms for classical X− >0 diffusion-reaction processes. FABRICE THALMANN, University of Strasbourg and Insitut Charles Sadron CNRS,Strasbourg,France, NAM-KYUNG LEE, Department of Physics, Sejong University, Seoul, South-Korea — The Doi formalism [J.Phys.A 9, p1465, 1976] treats a reaction-diffusion process as a quantum many-body problem. We use this second quantized formulation as a starting point to derive a numerical scheme for simulating X− >0 reaction-diffusion processes, following a well-established time discretization procedure. In the case of a reaction zone localized in the configuration space, this formulation provides also a systematic way of designing an optimized, multiple time step algorithm, spending most of the computation time to sample the configurations where the reaction is likely to occur.

K1.00160 Vibrational spectroscopic study of newly developed self-forming lipids and nanovesicles. RAJAN BISTA, REINHARD BRUCH, University of Nevada, Reno, Nevada, USA — We present the first experimental study of self-forming synthetic nanovesicles, trademarked as QuSomes\textsuperscript{TM}, using vibrational spectroscopic techniques namely near-infrared (NIR) and laser tweezers Raman spectroscopy. Raman spectra of these new artificial nanovesicles suspended in Phosphate Buffered Saline (PBS) have been obtained by using an inverted confocal laser-tweezer-Raman-microscopy system in the spectral range of 3100 to 500 cm\textsuperscript{-1}. This spectrometer works with an 80 mW diode-pumped solid-state laser, operating at a wavelength of 785 nm in the TEM\textsubscript{00} mode. The laser is used both for optical trapping and Raman excitation. Similarly, NIR absorption spectra of these novel nanovesicles have been recorded in the spectral range of 9000-4800 cm\textsuperscript{-1} by using a new miniaturized micro-mirror spectrometer based on micro-optical-electro-mechanical systems (MOEMS) technology. In this work, we have found that the most prominent bands in the studied spectral region of Raman spectra are dominated by vibrational modes arising from C-C and CH\textsubscript{2} bonds. Similarly, NIR spectra are primarily assigned as first and second overtone of C-H stretching mode and second overtone of C=O stretching mode. These spectroscopic techniques have proven to be an excellent tool to establish the fingerprint region revealing the molecular structure and conformation of QuSomes\textsuperscript{TM} nanoparticles.

K1.00161 Effects of Aggregation on the Properties of Individual Conjugated Oligomers and Polymers Probed by Fluorescence Microscopy. GIZELLE SHERWOOD, LINDA PETEANU, JURJEN WILDEMAN — The recent upsurge in use of conjugated polymers in photovoltaic devices and in displays drives the need for understanding how morphology affects important functional features such as emission and charge migration. Due to the inherent complexity of polymers, a parallel effort to ‘build-up’ understanding of their features via a detailed study of important electronic and photo-physical properties of oligomer aggregates is needed. These exhibit remarkably uniform spectral properties that defy analysis via standard exciton coupling models. Fluorescence microscopy is used to probe both variations in vibronic structure and emission lifetime between individual aggregates and trends in these properties as a function of aggregate size.

K1.00162 ARTIFICIALLY STRUCTURED MATERIALS —

K1.00163 Template assisted synthesis and optical properties of gold nanoparticles,\textsuperscript{1}. PETRU FODOR, VINCENT LA SALVIA, Cleveland State University — A hybrid nanofabrication method (interference lithography + self assembly) was explored for the fabrication of arrays of gold nanoparticles. To ensure the uniformity of the nanoparticles, a template assisted synthesis was used in which the gold is electrodeposited in the pores of anodized aluminum membranes. The spacing between the pores and their ordering is controlled in the first fabrication step of the template in which laser lithography and metal deposition are used to produce aluminum films with controlled strain profiles. The diameter of the pores produced after anodizing the aluminum film in acidic solution determines the diameter of the gold particles, while their aspect ratio is controlled through the deposition time. Optical absorbance spectroscopy is used to evaluate the ability to tune the nanoparticles plasmon resonance spectra through control over their size and aspect ratio.

\textsuperscript{1}This work was supported through a Cottrell College Science Award ID 7347 from the Research Corporation for Science Advancement.

K1.00164 Structural and Electrical Study of ZnO Nanowires Grown on Silicon and Titanium Substrates. EDWARD LIKOVICH, ERIC PETERSEN, VENKATESH NARAYANAMURTI, Harvard University School of Engineering and Applied Sciences — We studied the VLS (vapor-liquid-solid) growth of ZnO nanowires on catalytically patterned Silicon and Titanium foil substrates. We provide evidence for VLS growth from the formation of a eutectic liquid between Au catalyst particles and the Si or Ti substrate. In order to further understand conduction in nanowires, we present preliminary data from electrical measurements on wires grown on each substrate and provide a comparison. We show that the use of metal foil substrates exhibits promise for future nanowire applications in large-area light emitters, collectors, and thermoelectrics.

This work was supported through a Cottrell College Science Award ID 7347 from the Research Corporation for Science Advancement.
K1.00165 Electronic properties of boron nano-ribbons: - DFT study, SUMIT SAXENA, TREVOR A. TYSON, Department of Physics, New Jersey Institute of Technology, Newark, NJ. — Electronic properties of boron nano-ribbons have been studied using density functional techniques employing ultra-soft pseudo-potentials. Spin restricted calculations were performed for boron nano-ribbons constructed from stable boron sheet structures. Different stable edge configurations of nano-ribbons were observed. Band structure analysis was performed and Density of states was calculated to determine the electronic phase of these nano-ribbons. Comparisons with the carbon systems will be made. This work is supported in part by NSF DMR-051219.


K1.00166 Fundamentals of magneto-optics of single Rashba spintronic quantum dots, MANVIR KUSHWAHA, University of Puebla, Mexico — We report on the theoretical investigation of the effect of the Rashba-type spin-orbit interaction (SOI) on the Fock-Darwin energy spectrum in the parabolically confined quantum dots in the presence of a perpendicular [to the original two-dimensional electron gas (2DEG)] magnetic field. The study is based on the formal (analytical) results without resorting to any numerical simulation. We observe that the SOI modifies drastically the optical, thermodynamic, as well as magneto-optical properties of the (narrow-gap InAs) quantum dots. We discuss the dependence of the Fock-Darwin spectrum, Fermi energy, optical transitions, and magnetization on all the important parameters involved in the theory such as, for example, the orbital quantum number, the magnetic field, the confinement potential, and the Rashba parameter that characterizes the strength of the SOI. The illustrative examples include the results both with and without the SOI, for the sake of comparison. One of the most important observation is that the Rashba SOI causes the band mixing and band shifting in the quantum dots and the Fock-Darwin energy spectrum becomes richer but complex. This complexity seems to arise due to an intricate interplay between the SOI and the Zeeman energy.

K1.00167 Quantum Wire Fano Resonance in an Electric Field, V. VARGIAMIDIS, Aristotle University, Thessaloniki, Greece, V. FESSATIDIS, Fordham University, Bronx, USA, N.J.M. HORING, Stevens Institute of Technology, Hoboken, USA — Electronic transport through a straight parabolically confined quantum wire with an attractive impurity and a transverse electric field is investigated via the Feshbach coupled-channel theory. The impurity is modeled by a δ-function potential in the propagation direction while it is Gaussian in the transverse direction. In the presence of an impurity, the transmission probability of the wire may exhibit resonances of the Fano type (which is the result of the interference between background transmission and transmission via a quasibound state created in the impurity). It is shown here that increasing the field strength from zero causes displacement of the confining potential, thereby inducing a “shifting” of the impurity across the channel and therefore influencing the resonance structure. As the center of the confining potential approaches the center of the impurity, the coupling of the (first) propagating state with the quasibound state of the second channel gradually decreases, resulting in a decrease of the resonance width. For a particular value of the field strength the resonance width shrinks to zero and the Fano profile collapses. The resonance energy is also examined as a function of the electric field strength.

K1.00168 Fabrication and Electrical Characterization of Zinc Oxide Nanowires, DAQING ZHANG, CHUN-HONG LEE, CSU Fresno, CHRIS VERVEN, Univ. of Idaho, VANVILAI KATKANANT, CSU Fresno — One dimensional semiconducting zinc oxide (ZnO) nanowires have drawn attractive attentions in the past years. The unique electrical, optical, and piezoelectric properties of ZnO nanowires make them broad applications ranging from light emitting diode and lasers, solar cells, photodetectors, electron transporters and transistors, to piezoelectric generators. In our research, two-terminal current-voltage (I-V) measurements were conducted to determine the electrical conductivity alternation of the ZnO nanowires under laser irradiation, and various gaseous surroundings. The I-V curves at the temperature ranged from 150 to 300 K were recorded in vacuum. The Arrhenius plot shows perfect linear relation between I and T. The donor lever of the semiconducting nanowire is about 326 meV. We observed that the current increased by 50% with laser on in comparison to that with it off; it raised by a factor of four under ambient reductive gas CO. In addition, the I-V behaviors were found to be reversible with those various environments. Further studies on the possible nano-devices such as optical switches and chemical sensors are undergoing.

K1.00169 Elementary process of electromigration investigated by novel spectroscopic approach to electrical break junctions, Akinori Umeno, Kazuhiako Hirakawa, IIS, Univ. of Tokyo, INQIE TEAM, CREST-JST TEAM — We have investigated electromigration process at gold nanojunctions by introducing a novel spectroscopic analysis. Gold nanojunctions were broken into nanogaps by passing large current, which was controlled by monitoring the evolution of junction conductance. We observed that, for the junctions as small as few tens of atoms, the junction conductance showed successive drops by one quantum (e^2/h), corresponding to one-by-one removal of gold atoms, only when the junction voltage exceeded certain critical values. The histogram of the observed critical voltages showed a clear peak, V_p, and eV_p was found to agree with the activation energy for surface diffusion of gold atoms. The result indicates that the elementary process of electromigration in such small junctions is the self-diffusion of metal atoms driven by microscopic kinetic energy transfer from a single conduction electron to a single metal atom. Technological implications of this new finding are also discussed in terms of reproducible formation of nanogap electrodes for single molecular junctions and also failure-tolerant interconnections for VLSIs.

K1.00170 Band structure of core-shell semiconductor nanowires, MATS-ERIK PISTOL, Dept. of Solid State Physics, Lund University, Sweden, CRAIG PRYOR, Dept. of Physics and Astronomy, University of Iowa — We present band structures of strained core-shell nanowires composed of zincblende III-V (binary) semiconductors. We consider all combinations of AIN, GaN, InN, and all combinations of AIP, GaP, AIA, GaAs, InP, AlSb, GaSb, and InSb. We compute the Γ- and X-conduction band minima as well as the valence band maximum, all as functions of the core and shell radii. The calculations were performed using continuum elasticity theory for the strain, eight-band strain-dependent k·p theory for the Γ-point energies, and single band approximation for the X-point conduction minima. We identify structures with type-I, type-II and type-III band alignment, as well as systems in which one material becomes metallic due to a negative band-gap. We identify structures that may support exciton crystals with and without photocoexcitation. We have also computed the effective masses, from which the confinement energy may be estimated. All the results [Pistol and Pryor, Phys. Rev. B 78, 115319] are available in graphical and tabular form at www.semiconductor.physics.uiowa.edu

1M.E.P was supported by the Swedish Foundation for Strategic Research (SSF) and the Swedish Research Council (VR). C.E.P. acknowledges support from an NSF NIRT.

K1.00171 Analysis of electron transport through quantum dots using the Hidden Markov Model (HMM), MATTHEW HOUSE, HONG WEN JIANG, Department of Physics, University of California Los Angeles — The number of electrons present on a quantum dot defined in a two-dimensional electron gas in a semiconductor heterostructure can be observed using a nearby quantum point contact (QPC), but counting the number of electrons present in the dot does not directly reveal the presence of multiple allowed states that contain the same number of electrons; i.e. different orbital or spin states. Two or more states with the same number of electrons may have different rates of transition to other, directly observable states. In this case they may be indirectly distinguishable, by analysis of the statistics of a time series of data. We present a new approach to analysis of QPC data based on the Hidden Markov Model (HMM). HMM theory provides a mathematical framework for optimally estimating the rates of transition between a system with various states, which may include states that cannot be directly distinguished from one another by observation (they are “hidden”). Statistical tests can be applied to determine if the hypothesis of a “hidden” state is justified by the data. The application of the HMM framework to the quantum dot analysis problem and preliminary results of the application of this approach to electron transport data is presented.
K1.00172 Si$_{0.7}$Ge$_{0.3}$ Nanorings Mediated By Ag Nanodots: Structural Evolution and Enhanced Photoluminescence Properties

CHIN HO, CHENG-YING CHEN, JR-HAU HE, Natl Taiwan Univ, INSTITUTE OF PHOTONICS AND OPTOELECTRONICS TEAM — Currently nanorings (NRs) are attractive because there is a great deal of interest in nanostructures from theoretical, experimental, and device perspectives. The feasible NR fabrication is demanded in the field of electronic and optoelectronic devices at the nanoscale. In the present study, the growth of high-density Si$_{0.7}$Ge$_{0.3}$ NRs has been achieved on ultrathin Ag films on Si$_{0.7}$Ge$_{0.3}$ substrate. In situ ultrahigh-vacuum transmission electron microscopy revealed that the formation of nanorings involves a mechanism mediated by Ag NDs and evaporation of Ag-Si-Ge eutectic liquid at high temperature. Si$_{0.7}$Ge$_{0.3}$ NRs exhibit the enhanced PL intensity over Si$_{0.7}$Ge$_{0.3}$ thin film due to quantum size effects. The luminescence efficiency as a function of the size of Si$_{0.7}$Ge$_{0.3}$ NRs has been investigated. Power-dependent PL demonstrates that the NR mediated by Ag NDs is type-I band alignment. The process promising the availability of type-I Si$_{0.7}$Ge$_{0.3}$ NRs can serve as a useful platform for the fundamental understanding and future practical applications of NRs.

K1.00173 Experimental demonstration of reflection minimization at 2D photonic crystal interfaces via antireflection structures

TEUN-TEUN KIM, SUN-GOO LEE, MYEONG-WOO KIM, JAE-EUN KIM, HAE YONG PARK, Department of Physics, KAIST, 373-1 Guseong-dong, Yuseong-gu, Daejeon, Korea, PHOTONIC CRYSTAL LAB. DEPARTMENT OF PHYSICS, KAIST TEAM — We experimentally confirm that the antireflection structures effectively minimize the unnecessary reflections of self-collimated microwave beams in a two-dimensional square lattice photonic crystal composed of alumina rods. The optimized design parameters for the antireflection parameters are obtained from the one-dimensional antireflection coating theory and the finite-difference time-domain simulations. Measurements of the transmission through the photonic crystal samples with and without the antireflection coating structures agree well with the simulation results. Measured results show that the photonic crystal with an antireflection coating structure yields transmission of more than 80% of the incident power near the self-collimation frequency, which is more improved transmittance with wider band compared to the case without the antireflection coating structure.

K1.00174 Localized and Resonant elastic sagittal modes in one-dimensional phononic crystals

1, L. CASTRO-ARCE, Department of Research in Physics, University Sonora; Department Physics, Mathematics and Ingeering, unity Regional Sorth, Navojoa Sonora Mexico, F. RAMOS-MENDIETA, Department of Research in Physics, University of Sonora, Hermillos, Sonora Mexico — By incorporating a defect Zn layer in an Epoxy/Sn one-dimensional phononic crystal we found transmission peaks associated to localized longitudinal and transverse elastic states. The same localized modes of orthogonal polarizations are excited by incident longitudinal or transverse waves; thus, the transmission spectrum of localized vibrations does not depend on the polarization of the incident wave. The phenomenon can be explained on basis of mode conversion. In addition, resonant modes with frequencies lying inside a bulk band were also found. It is interesting that as function of both the size of the phononic sample and the angle of incidence, the polarization of the transmission resonant peaks change; for example, for a sample of seven cells with the defect at the center, the mode can change from quasitransverse to quasilongitudinal when the angle of incidence changes from 30 to 40 degrees. The variation of polarization is also independent of the polarization of the incident wave.

2The firt author has a scholarship from CONACYT (Mexico).

K1.00175 Transport Properties of Nanoscale Materials by First-principles Calculations


K1.00176 ThermoElectric and Structural Properties of Sintered LaCoO$_3$ Ceramics

1, A. CORTES, W. LOPERA, Thin Film Group Department of Physics, Universidad del Valle, Cali, Colombia, P. PRIETO, Excellence Center for Novel Materials — Electrical and thermal transport properties of LaCoO$_3$ in bulk are reported in the temperature range from 10 to 390 K. The crystalline structure of the samples was determined by x-ray diffractionometry (XRD). XRD measurements indicated that the formation of LaCoO$_3$ was completed, and it was verified that a pure phase with rhombohedral crystalline structure was obtained. The results of the thermoelectric measurements show that the Seebeck coefficient ($S$) initially grow with the increasing of temperature up to a maximum value around of 650 $\mu$V/K at 230 K. After this temperature $S$ decrease slowly up to a value of 520 $\mu$V/K, at room temperature. The polycrystalline LaCoO$_3$ samples show thermal conductivity around 0.4 W/mK at room temperature, that is a lower value than the reported for single crystal samples of this material. Electrical resistivity measurements show typical semiconducting behavior, with a large value of resistivity, close to 2.6 $\Omega$. Finally the thermoelectric figure of merit have a maximum value of 0.09, at room temperature, that is comparable to previous reported values for this material.

2This work has been supported by Colciencias under contract number RC 043-2005.

K1.00177 Accurate thermopower measurement of quasi-one dimensional nanomaterials

1, YI-BIN GAO, YE WANG, JUN-YI WANG, Department of Physics, Peking University, LIAN-MAO PENG, SHENG-YONG XU, Department of Electronics, Peking University — To measure accurate thermopower (Seebeck coefficient) of a nanomaterial is of importance for developing low-dimensional thermoelectrics and energy-conversion devices. We have built up sample stages with copper bulks and 25 micron-diameter gold wires, and assembled multi-wall carbon nanotubes (MWCNT) and individual nanowires onto these stages using in situ nano-probe manipulation in a scanning electron microscope. We can establish a temperature difference as high as 80K between two ends of a nanomaterial sample with this kind of stage, thus obtain a measurement accuracy of 2%-5%. For MWCNT bundles, we have observed a trend that, when the number of individual tubes in a bundle varies from several millions to around a thousand, the thermopower almost remains as a constant value around 10 microvolt per Kelvin. But when the tube number in the bundle is further reduced to less than a hundred, the thermopower increases steeply to a value near 20 microvolt per Kelvin. The result is attributed to the effect of surface adsorption of oxygen on the thermopower of the bundle.

3We acknowledge financial support from CNSF No 10774002 and CMST No 2006AA03Z350.
**K1.00178** Phonon Thermal Conductivity of Si/Ge Nanostructures, SHANG-FEN REN, Illinois State University. WEI CHENG, Beijing Normal University — Phonon thermal conductivities of various Si/Ge nanostructures (NSs), including nanocrystals, nanowires, nanowires, and Si/Ge nanocomposites, are investigated with three different models: macroscopic approximation, semi-microscopic model that calculates the heat capacity of NSs with a microscopic Valence-Force-Field Model (VFFM), and a full microscopic description of phonon thermal conduction that calculate both heat capacity and phonon group velocity by the VFFM. The results are compared, and the advantages and limitations of each of the models are discussed. It is shown that with full microscopic description, phonon thermal conductivity in Si/Ge nanostructures might be quite different from those obtained with the macroscopic description, mainly depending on the roughness of the interfaces and the size of the nanostructures. This further indicates that it is critically important to investigate phonon thermal conductivities in nanostructures with microscopic models when the roughness is important to consider and the size of the nanostructures is small.

**K1.00179** High Pressure Structural and Electrical Transport Properties of the Ca$_3$Co$_4$O$_7$ System, T. WU, T.A. TYSON, Z. CHEN, Department of Physics, New Jersey Institute of Technology, Q. JIE, Q. LI. Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, J.J. TU, Department of Physics. The City College of New York — High pressure and temperature dependent resistivity measurements were conducted on the Ca$_3$Co$_4$O$_7$ system to understand the influence of internal pressure by doping on the properties of these materials. To directly probe the effect of pressure on the structure, x-ray diffraction measurements under pressure were also conducted with diamond anvil cells at ambient temperature. The results are compared with ambient pressure chemically materials. The influence of the atomic structure on the thermolectric properties will be discussed.

**K1.00180** Magnetism in ZnO, CHANYONG HWANG, W. KIM, Korea Research Institute of Standards and Science, JISANG HONG, Department of Physics, Pukyung National University, H.J. KIM, Chungnam National University, Y.P. LEE, Department of Physicis and q-Psi, Hanyang University — DMS has drawn a lot of attention for the possible use in spintronics. Ferromagnetic order showed up after the doping the oxide such as ZnO with transition metals. The origin of this ferromagnetic order is still controversial. Especially addition of Cu as a dopant material for ferromagnetic order raises the question on the role of transition metal dopant for the existence of ferromagnetic order. We have used high energy electron beam to build the Zn vacancy. SQUID and MCD results will be presented for the existence of long range ferromagnetic order. First principles calculation also supports our model for the origin of this ferromagnetism. (Supported by KOSEF)

**K1.00181** Fabrication of Si nanowires on Si (100) using a scanning probe tip, JOSHUA SMITH, ROBERT DAVIS, YING YI DANG, GARY FEDDER, JIM BAIN, DAVID RICKETTS, Carnegie Mellon University — Reliable fabrication on the nanoscale is becoming increasingly important. The co-author team is investigating a nanolithography technique for the deposition of nanoscale features entitled “Tip-directed, field-emission assisted nanomanufacturing” (TFAN). The TFAN process involves the adsorption of a layer of silicon-containing gas, such as disilane, to a substrate and the selective patterning of the surface with field-emitted electrons from a scanning probe tip. The electrons crack the Si containing molecules, which results in the deposition of Si on the substrate. The adsorption of Si-containing molecules to the substrate surface is critical to the success of this approach. The investigation involves the determination of the coverage, sticking coefficient, and temperature constant of disilane on the Si(100) surface using temperature programmed desorption and scanning tunneling microscopy.

**K1.00182** Excitation energy dependence of fluorescence intermittency in CdSe/ZnS core-shell nanocrystals, ROBERT MOHR, THOMAS EMMONS, CATHERINE CROUCH, Swarthmore College — We report measurements of the excitation energy dependence of the fluorescence intermittency of single CdSe/ZnS core/shell nanocrystals (NCs) using two different excitation energies. The lower excitation energy, at 532 nm, corresponds to excitation of 270 meV above the band gap. The higher energy, at 405 nm, corresponds to excitation of 1.0 eV above the bandgap. At each excitation energy, 77 individual NCs were measured for 1500 s. The on-times from each individual NC follow a power-law distribution with the same exponent regardless of excitation energy. The on-times follow a truncated power law distribution with an exponent that is independent of energy, but the distribution of truncation times obtained from the individual NCs at the higher energy is peaked at shorter values than the distribution obtained with the lower excitation energy.

**K1.00183** Polarization-independent extraordinary optical transmission in three-dimensional metallic gratings, YUEHUI LU, MINHYUNG CHO, YOUNGPAK LEE, Hanyang University, Korea, JOOYULL RHEE, Sungkyunkwan University, Korea — Extraordinary optical transmission (EOT) is a unique effect that light is transmitted with an efficiency greater than unity when it is normalized to the area of grooves or holes. In this work, the EOT of both transverse-electric (TE) and transverse-magnetic (TM) polarizations was investigated for sub-wavelength metallic gratings by the rigorous coupled-wave analysis, implemented as the Airy-like internal reflection series. Generally, the EOT is achievable for TM polarization due to the excitation of coupled surface plasmon polaritons (SPPs), whereas the SPP-produced EOT for TE polarized light is impossible because of the absence of SPPs for this polarization. However, the TE-polarized EOT produced by cavity modes is available. In this work, the polarization-independent EOT is exhibited in the pure metallic gratings with broad slits without need for a specific dielectric filler in the grooves. The design proposed in this work simplifies the realization of gratings that possess the polarization-independent EOT.

**K1.00184** On Static and Dynamic Properties of Solitons in Molecular Chains, IRINA BARIAKHTAR, Boston College — The cross section for scattering of x-rays by solitons is calculated for the solitons corresponding to the formation of kinks in quasi-one-dimensional systems, e.g. molecular chains. Obtained is the temperature dependence of the soliton density, the shape of the particle density distribution in the soliton, based on the study of the x-ray scattering cross section by solitons, and other static and dynamic properties of the solitons in quasi-one-dimensional systems.

**K1.00185** SPP resonance and transmission enhancement of 1D slit array on aluminum film at microwave regime, MYEONG-WOO KIM, TEUN-TEUN KIM, JAE-EUN KIM, HAE YONG PARK, Department of Physics, KAIST, 373-1 Guseong-dong, Yuseong-gu, Daejeon, Korea, DEPARTMENT OF PHYSICS, KAIST TEAM — In this presentation, we show the transmission enhancement through periodically slit arrays on a metallic film experimentally measured in the microwave regime. Enhanced transmission peaks and sharp transmission dips are clearly observed near the surface plasmon polariton(SPP) resonance frequencies calculated theoretically. The measured transmittance spectra exhibit considerable dependence on the geometrical properties of slits such as slit width, slit periodicity and metallic film thickness. Transmission peaks and dips are originated from the coupling between the incident light and SPPs which are caused by the slit array which acts like a grating coupler. Obtained results are theoretically explained by solving the Maxwell’s equations and the diffraction theory with appropriate boundary conditions, which are in excellent agreement with those calculated by the finite-difference time-domain method.
Photoresponse in large area multi-walled carbon nanotube/polymer nanocomposite films, Paul Stokes, Jianhua Zou, Lei Zhai, Qun Huo, Saiful I. Khondaker, University of Central Florida, Nanoscience Technology Center, Department of Physics, Chemistry, Materials and Aerospace Engineering. Recently, photoresponse of CNTs (both in visible and near infrared (NIR) regime) have generated considerable debate in terms of whether the photoresponse is (i) due to photon induced charge carrier (excitonic), (ii) due to heating of the CNT network (bolometric), or (iii) caused by photodesorption of oxygen molecules at the surface of the CNT. In addition, the role of the metal electrode - CNT contact's effect on the photoresponse has also been debated. Here, we will present near IR photoresponse study of large area multi-walled carbon nanotube/poly(3-hexithiophene)-b-polystyrene polymer (MWNT/P3HT-b-PS) nanocomposite films for different loading ratio of MWNT in polymer matrix. We show that, compared to pure MWNT film, there is a large enhancement of photocurrent in MWNT/polymer composite film. The photocurrent strongly depends on the position of the laser spot with maximum response occurring at the metal - film interface. The time constant for the photoresponse is slow and varies between 0.6 and 1.2 seconds. We explain the photoresponse of the composite film by Schottky barrier modulation at the metal – film interface and discuss reasons for the slow time response.

Enhanced 1540 nm emission from ZnO:Er nanorod arrays via Ag island films, JIANG-WEI LO, CHIN-AN LIN, JR-HAUE HE, Natl Taiwan Univ. Self-assembled nanorod arrays (NRAs) heterostructures that consist of a single-crystalline Er-doped ZnO NRAs grown on Ag nanodot films have been synthesized by a chemical method and proposed as one of the promising optoelectronic materials since the Er intra-4f shell transition leads to 1540 nm emission for optical communication. The enhancement of 1540-nm emission of Er-doped ZnO NRAs via enhanced deep level emission of ZnO host resulted from local field enhancement effects of Ag nanodot films, and subsequent energy transfer to Er has been demonstrated. The microstructural analysis, electronic structure analysis, and photoluminescence characterizations have been performed to clarify the mechanism of enhanced 1540 nm emission. This paves the way to electrical pumping in a nano-system that forms NRAs of high-quality optical cavity.

Influence of Negative-Bias Voltage on Mechanical Properties of Quaternary Ti(Nb)(C)(N) Coatings, M.E. GOMEZ, J.C. CAicedo, C. AMAYA, G.A. MENDOZA, J. ALVARADO-RIVERA, J. MUNOZ-SALDANA, P. PRIETO, UNIVERSIDAD DEL VALLE, COLOMBIA TEAM, UNIVERSIDAD NACIONAL DE COLOMBIA, BOGOTA TEAM, CINVESTAV, IPN, QUERETARO, MEXICO TEAM, CENM, COLOMBIA COLLABORATION. Mechanical properties of quaternary Ti-Nb-C-N films via r.f magnetron sputtering process were studied by nanoindentation. The r.f. bias voltage was systematically varied from 0, -50, -100 V, keeping all other growth parameters fixed. Active vibration modes were analyzed by using Fourier transformed infrared spectroscopy (FTIR), where bands associated to Ti-N, Nb-C-N and Ti-C-N bonds, and to Ti-Nb-C-N stretching vibrations were found. Nanindentation results reaching the elastic-plastic behavior of the Ti-Nb-C-N films indicate that both hardness and elastic modulus increase from 22 to 30 GPa and from 220 to 306 GPa, respectively. Thus, increasing the bias-voltage from 0 to -100V a clear improvement of hardness and elastic modulus were obtained.

Electrical and Optical characterization of GaN$_x$As$_{1-x}$ fabricated using Ion Implantation and Pulsed Laser Melting, TAESEOK KIM, MICHAEL J. AZIZ, VENKATESH NARAYANAMURTI, School of Engineering and Applied Sciences, Harvard University, KIRSTIN ALBERI, National Renewable Energy Laboratory, OSCAR D. DUBON, Dept. of Materials Science and Engineering, University of California, Berkeley. We present a systematic investigation of the band structure of GaN$_x$As$_{1-x}$ alloys synthesized using nitrogen ion implantation followed by pulsed laser melting and rapid thermal annealing. The evolution of the nitrogen concentration-depth profile is consistent with liquid-phase diffusion, solute trapping at the rapidly moving solidification front, and surface evaporation. The reduction of the Schottky barrier height at nitrogen composition up to $x = 0.06$ is studied by ballistic electron emission microscopy (BEEM) and determined quantitatively using second voltage derivative (SD) BEEM spectra. This composition effect on the barrier height is consistent with the bandgap narrowing measured on the same samples by photomodulated reflectance and is also consistent with the band anti-crossing model for the splitting of the conduction band in GaN$_x$As$_{1-x}$ alloys. Lithographically patterned GaN$_x$As$_{1-x}$ dots are imaged by BEEM. Analysis of BEEM spectra from the locally confined dots indicates an alloying-induced decrease in the Schottky barrier height of four times the thermal energy at room temperature.

SURFACES, INTERFACES AND THIN FILMS

Ab-initio study of the O covered Cu(100), Cu(110), and Cu(111) surfaces, N.G. FAZLEEV, Department of Physics, University of Texas at Arlington. The study of adsorption of oxygen on transition metal surface is important for the understanding of oxidation, heterogeneous catalysis, and metal corrosion. The structures formed on transition metal surfaces vary from simple adlayers of chemisorbed oxygen to oxygen diffusion into the sub-surface region and the formation of oxides. In this work we present an ab-initio investigation of stability and associated physical and electronic properties of different adsorption phases of oxygen on Cu(100), Cu(110) and Cu(111) as well as of the clean Cu surfaces using density functional theory in the generalized gradient approximation and a four-layer slab to model the ideal Cu surfaces. In particular, we fully optimize the geometry of the surfaces with adsorbed oxygen and study the electronic structure, the changes in electron work function, surface energy, and interlayer spacings as a function of coverage. Furthermore, we study the chemistry of the metal-adsorbate bonding. Results and analysis are also presented for the Cu20(100) surface. We compare our results to both experimental data and other theoretical models.

Adsorption and Dissociation of Water on the (0001) Surface of DHCP Americium, PRATIK DHOLABHAI, ASOK RAY, The University of Texas at Arlington. Ab initio total energy calculations within the framework of density functional theory have been performed for water molecule adsorption on the (0001) surface of double hexagonal closed packed americium. Subsequent partial dissociation (OH-H) and complete dissociation (H=O-H) of the water molecule have been examined. The completely dissociated configuration exhibits the strongest binding with the surface followed by partially dissociated species, with all molecular H2O configurations showing weak physisorption. The change in work functions and net magnetic moments before and after adsorption will be presented for all the cases studied. The adsorbate-substrate interactions will be elaborated using the difference charge density distributions and the local density of states. The effects of adsorption on Am 5f electron localization-delocalization in the vicinity of the Fermi level will be discussed.
K.00193 Hydrogen adsorption on the (020) surface of α-Pu — A computational Study

RAY, MD ISLAM, University of Texas at Arlington, TX 76019 — We have studied the hydrogen adsorption on (020) surface of α-Pu and the effect of surface relaxation on chemisorption using relativistic full-potential augmented plane wave with local orbital basis method. The surface is modeled with four-layer slab consisting of 32 atoms with layer by layer anti-ferromagnetic arrangements. We have investigated the adsorption properties for four different adsorption sites, namely the top, the hollow, the short bridge and the long bridge sites. All the computations are carried out both at scalar relativistic level where spin-orbit interaction is ignored and where it is included, to study the effect of SO interaction on the adsorption properties. The effect of relaxation is also studied by calculating adsorption properties both on the relaxed and the non-relaxed surfaces. Our studies show that the short bridge is the most favorable site for hydrogen adsorption with chemisorption energy of 2.75 eV. Our study also shows that the spin-orbit coupling and the surface relaxation have very little impact on adsorption.

K.00194 Ab initio Calculation of optical properties of II-VI semiconductor surfaces

VAZQUEZ-NAVA, NORTERNO ARZATE, Centro de Investigaciones en Optica A. C., B.S. MENDOZA, Centro de Investigaciones en Optica — In this work we present some ab initio calculations of reflectance anisotropy spectra (RAS) of VI-II semiconductor surfaces having different surface reconstructions. We use an ab initio pseudopotential formalism in the framework of the density functional theory and within the local density approximation (DFT-LDA). We study the (001) polar surface of cadmium telluride (CdTe) and zinc telluride ZnTe with different reconstructions. Also we obtain RAS using a microscopic formulation based on a semi-empirical tight binding (SETB) approach which includes spin-orbit (SO) interactions [1]. We show RAS of each surface reconstruction and compare both theoretical results with experimental results [2]. We find a good agreement between experimental and theoretical spectra.


K.00195 Structure, composition and optical band gap of TiO₂ films prepared by d.c. magnetron sputtering

GOMEZ, A. ARIAS, E. CAMPS, L. ESCOBAR-ALARCON, F. ESPINOZA, J. MUÑOZ-SALDANA, G.A. MENDOZA, G. ZAMBRANO, UNIVERSIDAD DEL VALLE, COLOMBIA TEAM, INSTITUTO DE INVESTIGACIONES NUCLEARES (ININ), MEXICO TEAM, CINVESTAV, QUERÉTARO, MEXICO TEAM, UNIVERSIDAD NACIONAL DE COLOMBIA, BOGOTA TEAM — Titanium dioxide (TiO₂) thin films have been grown on silicon (001) substrate by d.c. magnetron sputtering. In an gas mixture at different Ar/O₂ ratio flow and at two different substrate temperatures (400 and 550 °C). Samples were characterized by X-ray diffraction, XRD, Raman spectroscopy, Scanning Electron Microscopy (SEM), Fourier Transformed Infrared Spectroscopy (FTIR) and UV-Vis analysis. Results showed that we obtained TiO₂-Anatase phase for the 90/10 of Ar/O₂ ratio in the gas mixture and at substrate temperature of 400 °C. The anatase phase proportion in the films decreases by increasing the oxygen concentration in the Ar/O₂ gas mixture. Optical band gap of 2.9 and 2.7 eV was calculated from UV-Vis spectra for sample grown at 90/10 and 80/20 of Ar/O₂ ratio, respectively.

Acknowledgments: This work has been partially supported by CENM-COLCIENCIAS contract 043-2005. Authors thank Department of Chemistry at Universidad del Valle for FTIR measurements.

K.00196 Growth and characterization of EuO thin films

BRENNER, M. EBLEN-ZAYAS, Carleton College — Eu-rich EuO is a ferromagnetic semiconductor that exhibits an insulator-metal transition associated with the onset of ferromagnetism and a colossal magnetoresistance response. In addition, the material is of interest for its possible use in spintronics. The materials properties are extremely sensitive to the stoichiometry of films. We will compare the properties of these films as a function of growth parameters, and discuss the stability of these films over time. In addition, we will present work comparing the properties of EuO thin films grown via reactive evaporation of Eu in the presence of an oxygen partial pressure with EuO films grown by Eu deposition followed by oxidation.

This work is supported by the Research Corporation and NSF DMR-0804715.

K.00197 Evolution of size distribution of Cobalt Silicide islands on (5x2) reconstructed Au/Si(111) surfaces

HUNG-CHIH KAN, TI-LI LIN, AN-LI CHIN, FU-KWO MEN, Department of Physics, National Chung Cheng University, Chia-Yi, Taiwan, ROC — We report our preliminary result on the observation of the evolution of Cobalt silicide islands on (5x2) reconstructed Au/Si(111) surfaces during high temperature annealing with snap-shot scanning tunneling microscopy (STM). At room temperature, we deposited Co on (5x2) reconstructed Au/Si(111) surfaces in an ultra-high vacuum (UHV) environment. We then annealed the surface at temperatures around 500 °C, and first observed the formation of cobalt silicide islands on the terraces and across the steps. Subsequent annealing causes the islands to evolve: the islands across the step continued to grow while those on the terraces eventually disappeared. The ripening process clearly favors the islands cross the steps. We developed our own image processing algorithm to segment the STM images scanned from the surface into individual islands and terraces. With that we analyze and compare the statistical trend of the evolution of the islands across the steps and that of those on the terraces.

This work is supported by the National Science Council, Taiwan, ROC.

K.00198 Atomic Modeling of the Grain Boundary in Silicon

MIZUSEKI, HIROSHI, SAHARA, RYOJI, KAWAZOE, YOSHIIKU, Institute for Materials Research, Tohoku University — By combining empirical potential approach with first-principles calculations, we investigate the atomic and electronic structures of grain boundary in silicon to estimate the deleterious effect on photovoltaic properties. Optimized geometries of several boundary structures are determined by using a Tersoff potential. Moreover, the electronic structures of boundary have been examined using the density-functional theory with the plane-wave pseudopotential method. Calculations show that the electronic properties depend strongly on the atomicistic structures, their properties are corresponding to efficiency of photovoltaic cell. This work was supported by the New Energy and Industrial Technology Development Organization (NEDO)
K1.00199 First principles study of Cu on Zn(0001): Resolution of the \((\sqrt{3} \times \sqrt{3})\)-R30° – Cu/ZnO(0001) surface phase, KAWATUT CHUASIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, BERNARD DELLEY, Paul-Scherer-Institut, CATHY STAMPFL, University of Sydney — The Cu/ZnO system is a well known catalyst for methanol synthesis as well as hydrogen production from methanol by the reverse water gas-shift reaction. Despite many years of effort to clarify the characterization and the synergetic mechanisms between Cu and ZnO, there still exists considerable novelty associated with the active phase of this combination catalyst. Recently, a \((\sqrt{3} \times \sqrt{3})\)-R30° phase has been reported on the Cu/ZnO(0001) surface (Dulub et al., Topics in Catalysis, 34, 65 (2005)). This reconstruction appears in the LEED pattern after annealing the pre-deposited Cu-clusters on the ZnO(0001) surface at 350 °C in a 10^-6 mbar O_2 environment for 10 minutes. In this work, we perform first-principles total-energy calculations within the framework of ab initio atomistic thermodynamics to investigate the atomic geometry and relative stability of this structure. We have extensively surveyed many possible atomic geometries, from which we are able to propose the atomic structure of this \((\sqrt{3} \times \sqrt{3})\)-R30° phase. To provide an overall understanding of this system, we also construct a two-dimensional phase diagram as a function of the Cu and O chemical potential, thus displaying the most stable surface structures.

K1.00200 Halomethane Adsorption on Graphite and Silica surfaces1, C. LAMSAL, G. LEUTY, Southern Illinois University at Carbondale, JONATHAN NEHRING, North Park University, MESFIN TSIGE, Southern Illinois University at Carbondale — Owing to their simple nature and number of practical applications, the adsorption of halomethanes onto various substrates has been a topic of study in materials science for a number of decades. While many studies have been directed towards the exploration of halomethanes as potential lubricant additives, the fundamental understanding of these compounds is still not well understood in general is the behavior of similar adsorbates on other, possibly widely different substrates. How the choice of substrate affects the manner in which these compounds are adsorbed as well as the effects of the substrate on the structure of the adsorbate more than a monolayer thick is less understood. In this presentation, we report the results of a recent molecular dynamics study comparing the structure and dynamics of systems composed separately of three tetra substituted halomethanes - CF3, CF2Cl, and CF2Br - adsorbed onto two different substrates - graphite and silica (α-quartz) - along a range of temperatures to examine how these systems evolve and change according to the characteristics of the substrate surface.

1Work supported by the Donors of the American Chemical Society Petroleum Research Fund.

K1.00201 Structure analysis and Physical property of Multiferroic LuFe2O4 Thin films, MINHWAN JUNG, SANGYOUN PARK, YOONHEE JEONG, POSTECH, Pohang, 790-784, S. Korea — Multi-ferroic materials have stimulated considerable interest because of technical applications in modern electronic devices such as memory elements and charge devices. LuFe2O4 was reported to have both ferrimagnetism and charge-ordering-induced ferroelectricity with the charge and spin frustrations. Since the material must be grown in thin film form before one would utilize the physical phenomena in practical applications, we have attempted to grow thin films of LuFe2O4. We have successfully obtained LuFe2O4 thin films on sapphire (0001) substrates by PLD method. Through XRD and PFMS measurements, their structure and magnetic property were characterized. In pole figure result, it showed 6 fold symmetry and there was a 30 degree rotation between the in-plane film and substrate direction. As for magnetic properties, we ascertained that the critical temperature was near 250K and it was identical to that of the bulk system.

K1.00202 Optical and structural analysis of In0.5−x,Ga,N alloys grown by HPCVD, GOKSEL DURKAYA, MAX BUEGLER, ENNO MALGUTH, Department of Physics & Astronomy, Georgia State University, WILL FENNICK, IAN FERGUSON, School of ECE, Georgia Institute of Technology, KONSTANTS E. DZIATK, Department of Physics & Astronomy, Georgia State University — The In0.5−x,Ga,N ternary alloy system has potential for development of high efficiency solar energy conversion and advanced optoelectronic device applications. InGaN hetero-structures of various compositions can be engineered to the responsive from UV to IR wavelength range, so that devices based on such heterostructures can cover the whole visible spectrum. However, the growth of such ternary In0.5−x,Ga,N alloys is challenging. This contribution focuses on the structural and optical characterization of In0.5−x,Ga,N layers and heterostructures grown by high pressure chemical vapor deposition (HPCVD), a growth technique that enables the stabilization of indium-rich In0.5−x,Ga,N alloys at elevated temperatures using 15 to 20 bar nitrogen overpressure. We will present the structural analysis of In0.5−x,Ga,N layers studied by Raman spectroscopy (RS), X-Ray Diffraction (XRD) and atomic force microscopy (AFM). The effects of composition and growth conditions on the layer surface topography and growth modes are studied by AFM.

K1.00203 Two Different Types of Single Crystal Morphologies of the γ-Phase and Their Conversion in Isotactic Polypropylene, YAN CAO, RYAN VAN HORN, CHI-CHUN TAI, MATTHEW GRAHAM, KWIANG-UN JEONG, CLAUDIO DE ROSA, BERNARD LOTZ, STEPHEN Z.D. CHENG — In the past, the crystallographic relationship between the γ-phase and the α-phase in isotactic polypropylene was extensively studied via oligomers of iPP. We attempt to investigate how the crystal morphological changes take place in the γ-phase using high molecular weight iPP-co-polystyrene samples. Due to the specific epitaxial growth of the γ-phase on the elongated α-phase single crystals, two different morphologies were identified via transmission electron and atomic force microscopies. The first γ-phase crystal morphology is needle-like. Selective area electron diffraction results showed that their [T10] or [110] zone axis was parallel to the thin film normal. The growth of this type of epitaxial γ-phase crystal was due to the step direction in the initial α-phase single crystal being parallel to the thin film normal. The second γ-phase crystal morphology was flat lamellae. This requires that the initial α-phase single crystal had to have a stem orientation tilted away from the thin film normal. Therefore, the sufficient and necessary condition for the γ-phase morphological conversion from the needle-like crystal to the flat crystal is the change of the stem orientation direction of the initial α-phase single crystals.

K1.00204 Reactive properties of chemically modified Pd(100) surface revealed by Kinetic Monte Carlo simulations, DOMINIC ALFONSO, National Energy Technology Laboratory — The interaction of H2 and CO with sulfur-covered Pd(100) surface represents a prototype model for understanding the various reasons for the poisoning of palladium by sulfur compounds. The use of Kinetic Monte Carlo method to investigate this system was explored. A Kinetic Monte Carlo code was developed and used to monitor the hosts of competing elementary steps associated with the adsorption, diffusion and desorption of H2 and CO on the metal surface. The input parameters such as rate of reactions and lateral interactions were obtained from density functional theory calculations within the generalized gradient approximation. We demonstrate that Kinetic Monte Carlo simulation is a powerful tool for elucidating the microscopic details of the behavior of H2 and CO on the poisoned surface.

K1.00205 Adsorption of Dimethyl Disulfide (DMDS) on a Metallic Quantum Well System, LEVAN TSISKURITI, SYLVIE RANGAN, ROBERT BARTYNSKI, Rutgers University — We have studied the bonding of the thiol molecule dimethylsulfide (SC(H)2)2 on ultrathin Cu films that exhibit metallic quantum well (MQW) states using inverse photoemission (IPE), reflection-absorption infrared spectroscopy (RAIRS) and temperature programmed desorption (TPD). This thiol is similar to more complex organic molecule which exhibits the self-assembled properties on metal surfaces. After a room temperature exposure of the Cu surface to the thiol molecule at a dose of ~ 2.5 L, a c(2 x 2) low energy electron diffraction (LEED) pattern confirmed that the adsorbate forms an ordered overlayer. A large sulfur signal is observed in Auger electron spectroscopy (AES) and the C-H stretch mode was observed in IR with a frequency of 2915 cm^-1 confirming molecular adsorption. Changes in the IPE spectrum upon adsorption are dominated by suppression of the substrate-related features, although some weak adsorbate-induced peaks are also observed. Both experimental and theoretical evidence indicates that the bonding of this thiol molecule is characterized by the formation of the C-S bond with the Cu substrate. The position of the C-S bond in the LEED pattern shows the self-assembled properties of the thiol molecule will be discussed.
K1.00206 Surface-state Emission of Si(111)-(7x7) Induced by Scanning Tunneling Microscopy

Hiroshi Imada, Masashi Ohta, Naoki Yamamoto. Condensed Matter Physics, Tokyo Institute of Technology — The luminescence measurement method we employ which utilizes a phenomenon called scanning tunneling microscope light emission (STM-LE) enables us to investigate surface structures with atomic resolution. However, STM-LE has not been well established, because the involved physics leaves many problems to be solved. In the present work, we studied STM-LE from Si(111)-7x7 surface to elucidate the nature of STM-LE of semiconductor surface. All the experiments were performed in an UHV-STM. Ag-covered Mo tips were used. Photon mapping and spectral measurement were performed. Emission spectra of Si(111)-7x7 at both bias polarities show very similar shape and behavior. The peaks are at 1.4eV, 2.3eV and around 1.6eV and do not shift with applied voltage. Since the position of the peak around 1.6eV shifts with tip shape but those of the 1.4eV and 2.3eV peaks are intrinsic to Si(111)-7x7 surface. Whole emission mechanism includes excitation of localized surface plasmon (LSP), excitation and decay (light emission) of surface electron and enhancement of the light. The photon maps show so high spatial resolution that individual adatoms can be clearly recognized.

K1.00207 Confined states in metallic thin films analyzed with a one-dimensional-pseudo-potential approach

Dah-Ann Luh, National Central University, Cheng-Maw Cheng, Ku-Ding Tsuei, National Synchrotron Radiation Research Center, Jian-Ming Tang, University of New Hampshire — An approach based on a one-dimensional pseudo-potential (1DPP) is proposed to analyze the confined states in metallic thin films. The potential of a thin-film system near the Fermi level is approximated with a pseudo-potential that is constructed with periodic potentials in the substrate and the film and with an image potential in the vacuum. The confined states are obtained by solving the Schrödinger equation. The result from applying the 1DPP approach to analyze the bound states in Ag/Au(111) thin films will be presented.

K1.00208 ABSTRACT WITHDRAWN

K1.00209 A First Principles Study of the Adsorption and Dissociation of CO2 on the δ-Pu (111) Surface

Raymond Atta-Fynn, Asok Ray. Department of Physics, The University of Texas at Arlington — Ab initio calculations within the framework of density functional theory have been used to study the adsorption of molecular CO2 and the corresponding partially dissociated (CO+O) and completely dissociated (C+O+O) products on the δ-Pu (111) surface. The completely dissociated C+O+O configurations exhibit the strongest binding with the surface (5.85 eV), followed by partially dissociated products CO+O (4.34 eV), with molecular CO2 adsorption having the lowest binding energies (2.98 eV). For all initial vertically upright orientations the CO2 molecule is physisorbed and its geometry and orientation does not change. For all initial flat lying orientations chemisorption occurs, with the final state corresponding to a bent CO2 molecule with bond angles of 118°-130° except one case where spontaneous partial dissociation from the atop site occurs. The interactions of the CO2 and CO with the Pu surface have been analyzed using the energy density of states and different charge density distributions.

K1.00210 Delta zeta: Improvement of the reproducibility of zeta potential measurements by transformation

Danish Faruqui, Paul J. Sides, Andrew J. Gellman. Carnegie Mellon Univ — When measuring the zeta potential of planar substrates as a function of pH, the results sometimes varied day by day even for the same sample treated exactly the same way. The shapes of the titration curves, however, were consistent despite apparent offsets. When data acquired on fused silica were transformed by subtracting the zeta potential measured at the initial condition from each subsequent measurement, however, data from many experiments fell on the same curve with a much reduced variance. Examination of the fundamental relationship between charge density and the zeta potential, derived from the Gouy Chapman theory of the electrical double layer, revealed that subtraction of the initial datum from each subsequent point amounted to cancellation of the total number of ionizable sites from the measurement. The transformed data reflected only chemical information such as equilibrium constants and activities. The principle assumptions are that the number of ionizable sites are fixed during a given experiment and the zeta potential magnitude is 100 mV or higher. Model expressions were verified for different mineral surfaces in range of aqueous solutions.

K1.00211 Operando Positron Annihilation Gamma Spectrometer (OPAGS)

S. Satyal, K. Shastry. University of Texas at Arlington, S. Mukherjee, University of Texas at Arlington, A.H. Weiss. University of Texas at Arlington — Surface properties measured under UHV conditions cannot be extended to surfaces interacting with gases under realistic pressures due to surface reconstruction and other strong perturbations of the surface. Surface probing techniques require UHV conditions to perform efficiently and avoid data loss due to scattering of outgoing particles. This poster describes the design of an Operando Positron Annihilation Gamma Spectrometer (OPAGS) currently under construction at the University of Texas at Arlington. The new system will be capable of obtaining surface and defect specific chemical and charge state information from surfaces under realistic pressures. Differential pumping will be used to maintain the sample in a gas environment while the rest of the beam is under UHV. Elemental content of the surface interacting with the gas environment will be determined from the Doppler broadened gamma spectra. This system will also include a time of flight (TOF) Auger spectrometer which correlates with the results of the Doppler measurements at lower pressures. By employing the unique capabilities of OPAGS together with those of the TOF PAES spectroscopy the charge transfer mechanisms at the surface in catalytic systems can be understood.

K1.00212 Temperature Programmed Desorption Study of Dodecanethiol Self-Assembled Monolayers on Ag

Simona Riemann, Nicholas Clark, Jennifer Walters, Daniel Field, Heike Geisler, Carl Venticello. Texas State University — The desorption kinetics of dodecanethiol self-assembled monolayers grown on Ag films has been studied using temperature programmed desorption. The self-assembled monolayers have been grown either in solution or by vapor deposition in UHV. The direct detection of dodecanethiol by the residual gas analyzer gives a complex spectrum due to multiple cracking fragments that are produced during the ionization of the molecule. The temperature programmed desorption measurements indicate that desorption of the self-assembled monolayer occurs in a two-stage process: dissociation of the alkane chain followed by desorption of the sulfur from the surface. Alkane chain fragments other than methane are observed to desorb over a range of ~150°C to ~220°C. Methane desorption starts at ~100°C and persists to ~350°C. In addition, the desorption of sulfur is observed starting at ~220°C.
K1.00213 Terpyridine Monolayer FETs as models for charge transport

K1.00214 Ordered Co Clusters On Boron-Nitride Template Layers

K1.00215 A Theoretical Study of the Graphite Surface Patterns

K1.00216 Temperature and Interlayer Control of Schottky Barrier Height

K1.00217 Quantifying Polarization at Peptide-Gold Interfaces Due to Mirror Charges

K1.00218 ATOMIC, MOLECULAR AND OPTICAL (AMO) PHYSICS

K1.00219 Ground state of the hydrogen negative ion

K1.00220 Electric Field-enhanced Intermolecular Bonding: an Ab Initio Density Functional Investigation

1University of Pittsburgh

1Supported by National Science Foundation DMR-0706138

1Supported by NERSC Arkansas-Oklahoma.
K1.00221 Charge Exchange in Slow Collisions of O+ with He — L.B. ZHAO, D.C. JOSEPH, B.C. SAHA, Department of Physics, Florida A&M University, Tallahassee, FL-32307, H.P. LEBERMAN, P. FUNKE, R.J. BUENKER, Bergische Universität Wuppertal, D-42097 Wuppertal, Germany — A comparative study is reported for the charge transfer in collisions of O+ with He using the fully quantal and semiclassical molecular-orbital-coupling (MOCC) approaches in the adiabatic representation. The electron capture processes O+→(1S0, 2D0, 3P0) + He → O(1P0) + He+ are recalculated. The semiclassical MOCC approach was examined by a detailed comparison of cross sections and transition probabilities from both the fully quantal and semiclassical MOCC approaches. The discrepancies reported previously between the semiclassical and the quantal MOCC cross sections may be attributed due to the insufficient step-size resolution of the semiclassical calculations. Our results are also compared with the experimental cross sections and found good agreements. This work is supported by NSF, CREST program (Grant#0630370).

K1.00222 K-Shell Ionization of Neutral Targets by Electron Impact — A.K.F. HAQUE, M.S.R. SARKER, M.A.R. PATOARY, M. SHAHJAHAN, M.I. HOSSAIN, M.A. UDDIN, A.K. BASAK, Department of Physics, University of Rajshahi, Bangladesh, B.C. SAHA, Department of Physics, Florida A&M University, Tallahassee, FL-32307. — The electron impact K-shell ionization cross sections (EIKICS) are needed in diverse fields, such as plasma-, radiation-, astrophysics. For plasma modeling the demand of EIKICS is enormous; this can only be fulfilled by simple analytical or semi-classical models that can generate efficiently accurate results over wide ranges of projectile energies and target species. We modified the Deutsch-Mark [1] model by incorporating ionic and relativistic corrections and applied to evaluate K-shell ionization cross sections for 30 atomic targets, 1Z<92 for 1<Z<2 GeV with very encouraging results as compared to available experimental findings. Work is supported by NSF, CREST project.


K1.00223 Gold cluster beyond hollow cage: Double-shell Au58 — CHUAN-DING DONG, XIN-GAO GONG, Fudan University, Shanghai, PR China — Gold clusters were found to have planar and hollow cage-like structures due to the strong relativistic effect. By using first principles calculation, we take Au58 as an example to demonstrate that gold cluster can show shell structure. Au58 reaches its highest stability with an optimal inner core of 10 atoms. Particularly, a double-shell structure with a hollow inner shell shows remarkable robustness. It is significant to consider this shell structure as a descendant of the hollow cage structures found previously, such as tetrahedral Au40, icosahedral Au122, tubular Au183 and so on, for this implies a possible evolution from planar, to cage, to shells and finally to the compact structure as the number of atoms in the cluster increasing.

K1.00224 An Investigation of Methanol Transitions at Cold Temperatures through Collisonal Cooling — KELLY SALB, DANIEL WILLEY — The detection of molecular transitions in the interstellar medium (ISM) has long been of interest to astrophysicists. If molecules and their interactions can be understood, then scientists may better understand the workings of space such as star formation. Methanol, CH3OH, has long been detected by astrophysicists in the ISM as an important constituent with a rich spectrum as a result of its asymmetry and that its low-energy torsional vibrations of the methyl group against the OH top can be excited under interstellar conditions. We investigate collisions of methanol with helium, a prominent constituent of the ISM, at temperatures between 5-30K through spectroscopy to better understand the interaction in the ISM.

K1.00225 Non-Linear Interactions in Pump-Probe Optical Phenomena1 — VERNE JACOBS, Naval Research Laboratory — Reduced density matrix descriptions are developed for pump-probe optical phenomena in atomic systems, taking into account atomic collisions as environmental phenomena. Time-domain (equation-of-motion) and frequency-domain (resolvent- operator) formulations are developed in a unified manner. In a semiclassical perturbative treatment of the electromagnetic interaction, compact Liouville-space operator expressions are derived for the linear and the general (n'th order) non-linear electromagnetic-response tensors. These expressions are valid for coherent atomic excitations and for the full tetradic-matrix form of the collision operator in the Markov approximation.

K1.00226 Efficient and Selective Photon Detection using Amplification Without Inversion.1 — KEVIN MERTES, MICHAEL DI ROSA, Los Alamos National Laboratory — We describe ongoing theoretical and experimental research at Los Alamos National Laboratory of a new technology for photon detection that exploits quantum processes to attain an unrivaled combination of high quantum efficiency and sharp discrimination. The amplification without inversion (AWI) scheme we are exploring consists of a Λ system found in the excited states of 264Hg. The 63P0 ⇒ 1 and 63P2 ⇒ 2 states form the lower 2 levels of the Λ system, and 73S1 ⇒ 3 forms the upper level. By incoherently pumping Hg vapor into [3] while simultaneously driving [3] ⇒ [2], approximatly 50% of the population will reside in [1]. Under these conditions, the system is radiating along [3] → 1 with an emission spectrum with a narrow dark line centered precisely on the [3] → 1 resonance. A faint light signal that is resonant with the [3] ⇒ 2 transition that enters the system would precipitate a coherent pulse of photons. This gain occurs from the coherent redistribution of population through level [3]. The expected spectral width for gain is a narrow 20 MHz. Due to spontaneous-emission quenching the noise added from this scheme should be significantly less than ordinary laser amplifiers.

1Work supported by the Office of Naval Research and the Defense Advanced Research Projects Agency.

K1.00227 Improved test of the standard model of elementary particles with atomic parity violation1 — KYLE BELOY, Univ. of Nevada, Reno, SERGEY PORSEV, Petersburg Nuclear Physics Institute, ANDREI DEREVIANKO, Univ. of Nevada, Reno — Atomic parity violation places powerful constraints on new physics beyond the Standard Model (SM) of elementary particles. The measurements are interpreted in terms of the nuclear weak charge, quantifying the strength of the electroweak coupling between atomic electrons and quarks of the nucleus. We report the most accurate to-date determination of this coupling strength by combining previous measurements by the Boulder group with our high-precision calculations in cesium atom. Our result is in a perfect agreement with the prediction of the SM. In combination with the results of high-energy collider experiments, our work confirms the predicted energy dependence (or “running”) of the electroweak interaction over an energy range spanning four orders of magnitude (from ∼10 MeV to ∼100 GeV) and places new limits on the masses of extra Z bosons (Z′). Our raised bound on the Z′ masses carves out a lower-energy part of the discovery reach of the Large Hadron Collider. At the same time, a major goal of the LHC is to find evidence for supersymmetry (SUSY), one of the basic, yet experimentally unproven, concepts of particle physics. Our result is consistent with the R-parity conserving SUSY with relatively light (sub-TeV) superpartners. This raises additional hopes of discovering SUSY at the LHC.

1Work supported by NIST, NSF, and RFBR.

K1.00228 Micromagic clock: microwave clock based on atoms in an engineered optical lattice — KYLE BELOY, ANDREI DEREVIANKO, Univ. of Nevada, Reno, VLADIMIR DZUBA, VICTOR FLAMBAUM, Univ. of New South Wales, Sydney — We propose a new class of atomic microwave clocks based on the hyperfine transitions in the ground state of aluminum or gallium atoms trapped in optical lattices. For these elements magic wavelengths exist at which both levels of the hyperfine doublet are shifted at the same rate by the lattice laser field, cancelling its effect on the clock transition. This work represents an elegant piece of theoretical physics containing a challenge to the experimentalist to realize a new frequency standard based on these proposed clocks.

1Fundings are provided from the Laboratory Directed Research and Development program of the Los Alamos National Laboratory.
K1.00220 Precession in Atomic Mechanics , ALFRED PHILLIPS, JR., Source Inst / Cornell U — With Atomic Mechanics we have been able to accurately calculate the measured values of the NIST He I and He II energy levels. Our model requires much less mathematical tedium than does the Schrödinger method but with equal accuracy. We made the conjecture that the angular momentum for excited electrons is \( n + \delta n \) h-bar. We had hypothesized that the delta \( n \) was a fractal. We have subsequently found a more conventional quantum mechanical explanation for delta \( n \). We model the delta \( n \) by assuming that the excited electron undergoes precession with a quantum number, \( l \), having values of 1, 2, 3, . . . . We will discuss the precession model. We expect that our model may be used in calculating the spectra of more complex atoms, lithium onward, that have been formillable mathematically using the Schrödinger theory.

K1.00230 COLD GAS —

K1.00231 Faraday patterns in interference experiments with one dimensional gases of ultracold atoms , SUSANNE PIELAWA, VLADIMIR GRITSEV, EUGENE DEMLER, Harvard University — We analyze a quantum analogue of the Faraday instability in one dimensional ultracold gases. Temporal periodic modulation of the interaction strength parametrically excites collective modes and gives rise to standing wave patterns in interference experiments. We discuss both bosonic and fermionic systems and demonstrate that such experiments can be used to probe spin charge separation.

K1.00232 Phase Separation in Bose-Superfluid Fermi Mixtures , B. RAMACHANDRAN, S.G. BHONGALE, H. PU, Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, TX 77005, USA — We study the phase diagram of 3-dimensional mixtures of BEC and a two-component superfluid fermi gas, referred to as Bose-Superfluid fermi mixtures, at zero and finite temperature. At zero temperature, we identify regimes at equilibrium in which the mixture exists either as a pure superfluid phase coexisting with a mixed phase or as a single homogenous phase. We identify critical boson densities at which phase separation occurs for different values of the fermi-fermi interaction strength. As a potential application of this phase separation phenomenon, we consider BEC to be in a realistic cigar-shaped double-well trap acting as a probe of the superfluid state. We show that the critical boson densities obtained from the phase diagram can be used to map the spatial density profile of the bosons using Local Density Approximation (LDA) in the trap setting. We show a methodology to robustly detect the “local” value of the superfluid Gap parameter by observing the boson density profile in the trap. We also explore the more challenging problem of phase separation in these mixtures at finite temperature. We show that, under proper conditions, this spatial phase separation phenomenon occurring in the presence of the BEC probe can be used to potentially detect the onset temperature of the BCS superfluidity.

K1.00233 Fermionic quantum gases with tunable interactions in optical lattices , ULRICH SCHNEIDER, LUCIA HACKERMÜLLER, Universität Mainz, Germany, THORSTEN BEST, SEBASTIAN WILL, SIMON BRAUN, MARIA MORENO CARDONER, BELEN PAREDES, Universität Mainz, IMMANUEL BLOCH, Universität Mainz, Max Planck Institut für Quantenoptik, Garching, Germany — Fermionic atoms in optical lattices can serve as a model system for condensed matter physics, as they present an implementation of the Hubbard hamiltonian with high experimental control of the relevant parameters. In our system we sympathetically cool \( ^{87}\text{Rb} \) and \( ^{40}\text{K} \) in an optically plugged quadrupole trap and an optical dipole trap. After evaporation, a balanced spin mixture of \( 40\text{K} \) atoms is loaded into a blue detuned optical lattice where the interactions can be changed via a Feshbach resonance. We present experimental and theoretical studies of the behaviour of fermionic atoms for both attractive and repulsive interactions. For repulsive interactions we show a transition from compressible, metallic states to Mott-insulating and finally band insulating states. On the attractive side we investigate an anomalous expansion when the interaction is strongly attractive and study the dynamics of atoms and repulsively and attractively bound pairs.

K1.00234 Interacting Mixtures of Bosons and Fermions in Optical Lattices , SEBASTIAN WILL, THORSTEN BEST, SIMON BRAUN, ULRICH SCHNEIDER, LUCIA HACKERMÜLLER, IMMANUEL BLOCH, Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — Mixtures of ultracold atomic quantum gases in optical lattices form novel quantum many-body systems offering unique controllability. In particular, degenerate Bose-Fermi mixtures have only recently come into experimental reach and are the topic of fruitful theoretical investigation. Among the most prominent predictions are the formation of charge-density waves, polaron-like quasi-particles and even supersolid ordering. We have prepared a mixture of bosonic \( ^{87}\text{Rb} \) and fermionic \( ^{40}\text{K} \) in a 3D optical lattice potential and investigated its properties depending on the interspecies interaction. We found a marked shift in the superfluid to Mott-insulator transition and were able to fully explain our findings in terms of an effective Bose-Hubbard model, employing renormalized Hubbard parameters. In recent measurements of the absolute intra- and interspecies interaction energies on individual lattice sites, we were able to further elucidate the effects of interaction in the optical lattice a thorough understanding of which may be an important step on the way towards complex quantum many-body states.

K1.00235 Spin-imbalance of ultracold Fermions in quasi-1D1, 2, ANN SOPHIE C. RITTNER, YEAN-AN LIAO, WENHUI LI, TOBIAS PAPROTTA, RANDALL G. HULET, Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77005 — After the success of BCS theory, more exotic forms of superfluidity have generated large interest in the condensed matter and cold atoms community. One prominent example is the elusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase, a polarized superfluid that is predicted to occur when superconductors are subjected to a strong magnetic field. At present, there is no experimental evidence for the FFLO phase in a 3D system, but it is predicted to occupy a larger region of the phase diagram in a quasi-1D system. We have implemented a 2D optical lattice in order to explore the phase diagram of a quasi-1D polarized Fermi gas.

1 Work supported by NSF, DARPA, ONR, and the Welch and Keck foundations.


K1.00236 Wavepacket Dynamics in Energy Space of a Chaotic Trimeric Bose-Hubbard System , MORITZ HILLER, Department of Physics, Albert Ludwigs University of Freiburg, Germany, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown CT-USA and MPI for Dynamics and Self-Organization, Goettingen-Germany , THEO GEISEL, MPI for Dynamics and Self-Organization, Goettingen-Germany — We study the energy redistribution of interacting bosons in a ring-shaped quantum trimer as the coupling strength between neighboring sites of the corresponding Bose-Hubbard Hamiltonian undergoes a sudden change \( \delta \). In the framework of (ultra-)cold atoms on optical lattices this perturbation corresponds to a modulation of the trapping potential height. Our analysis is based on a three-fold approach combining linear response theory calculations as well as semiclassical and random matrix theory considerations. The \( \delta \)-borders of applicability of each of these methods are identified by direct comparison with the exact quantum mechanical results. We find that while the variance of the evolving quantum distribution shows a remarkable quantum-classical correspondence (QCC) for all \( \delta \)-values, other moments exhibit this QCC only in the non-perturbative \( \delta \)-regime.
Quantum nucleation and macroscopic quantum tunneling in cold-atom boson-fermion mixtures

Dmitry Solenov, Dmitry Mozrytsky, Theoretical Division, Los Alamos National Laboratory

We present the results on kinetics of phase separation transition in boson-fermion cold atom mixtures. The parameters at which the transition is governed by quantum nucleation mechanism are identified. We demonstrate that for low fermion-boson mass ratio the density dependence of quantum nucleation transition rate is experimentally observable. The crossover to macroscopic quantum tunneling regime is analyzed. Based on a microscopic description of interacting cold atom boson-fermion mixtures we derive an effective action for the critical droplet and obtain an asymptotic expression for the nucleation rate in the vicinity of the phase transition and near the spinodal instability of the mixed phase. We show that dissipation due to excitations in fermion subsystem play a dominant role close to the transition point.

Quantum information, concepts, and computation

Quantum manipulation of low-frequency fluctuators with a superconducting resonator

Lin Tian, School of Natural Sciences, University of California, Merced, CA 95344, Kurt Jacobs, Department of Physics, University of Massachusetts at Boston, 100 Morrissey Blvd, Boston, MA 02125 USA

Spurious two-level systems (fluctuators) in superconducting devices have demonstrated long coherence time and can be considered as qubits instead of sources of decoherence. Coherent coupling between two-level system (TLS) and superconducting phase qubit has been observed in experiments. Here, we show that universal quantum logic gates on the TLS qubits can be implemented via the coupling between the TLSs and a superconducting microwave resonator in a cavity QED setup. By adjusting the driving on the resonator mode, parameters of individual TLS can be controlled to realize single qubit gates. Meanwhile, effective coupling can be generated between TLSs via their simultaneous coupling to the resonator mode. We present concrete designs for the gate operations and our numerically simulation shows that high fidelity can be achieved for the gate operations in the presence of resonator decay even at decay rates of a few megahertz. The nonlocal nature of the resonator mode also makes the TLSs intrinsically scalable for testing quantum algorithms.

Higher Energy Levels in Qubit Networks

Zechariah Thrailkill, Joseph Lambert, Roberto Ramos, Drexel University

Josephson junctions can be capacitively coupled together to form qubit networks capable of carrying out quantum logic operations. In order to fully utilize these systems, the influence of energy levels higher than the ground and first excited states in the qubits must be examined. We have analyzed such networks with three, four, and more qubits biased to both anharmonic and harmonic regimes. As the qubits become harmonic, the higher energy levels will interact more strongly with the computational basis. Allowing the system to pass through these higher energy levels can allow quantum state transfers where, in the anharmonic regime, it would not occur. We will discuss the impact these higher energy levels have on the natural state evolution of the systems, quantum information transfer, and state manipulation using a time independent, or adiabatically changing Hamiltonian.

Quantum hacking: Experimental demonstration of time-shift attack against practical quantum-key-distribution systems

Yi Zhao, Chi-Hang F. Fung, Bing Qi, Christine Chen, Hoi-Kwong Lo, Center for Quantum Information and Quantum Control, Department of Physics and Department of Electrical & Computer Engineering, University of Toronto

We have demonstrated the applicability of ground-state and time-dependent density functional theory to quantum computing systems by proving the Hohenberg-Kohn and Runge-Gross theorems for a fermion system representing N qubits. Time-dependent density functional theory is used to determine the minimum energy gap Δ(N) arising from application of the quantum adiabatic evolution algorithm to the NP-Complete problem MAXCUT. As density functional theory has been used to determine the minimum energy gap for a quantum gas microscopic to experimentally realize high resolution imaging and spatial addressability of a rubidium atom ensemble loaded into an optical lattice. Very good optical access to the atoms combined with solid immersion-like geometry is expected to provide an imaging resolution of about 0.5 microns. We realize a long lived two-dimensional quantum gas inside a novel opto-magnetic surface trap using an evanescent wave potential. To create the lattice potential we developed a projection approach using holographic phase masks. We have loaded a quantum gas into the lattice potential and are working on resolving single atoms on the lattice sites.

Efficient local implementation of bipartite nonlocal unitaries

Li Yu, Robert Griffiths, Carnegie Mellon University, SCOTT COHEN, Duquesne University

By definition, nonlocal unitaries cannot be implemented locally. However, if spatially separated parties share nonlocal resources (i.e., entanglement), they may be able to implement a nonlocal unitary by performing only local operations and sharing classical information. We provide protocols for doing so, which generalize previously published methods and in many cases allow tasks to be accomplished with fewer nonlocal resources than is required when using teleportation. We also discuss our insight into how and why entanglement allows such a task to be accomplished, an insight which arises from a diagrammatic approach allowing one to picture the processing of quantum information.

Density functional theory and quantum computation

Frank Gaitan, Southern Illinois University, FRANCO NORI, RIKEN/University of Michigan

We present our implementation of a quantum gas microscopic to experimentally realize high resolution imaging and spatial addressability of a rubidium atom ensemble loaded into an optical lattice. Very good optical access to the atoms combined with solid immersion-like geometry is expected to provide an imaging resolution of about 0.5 microns. We realize a long lived two-dimensional quantum gas inside a novel opto-magnetic surface trap using an evanescent wave potential. To create the lattice potential we developed a projection approach using holographic phase masks. We have loaded a quantum gas into the lattice potential and are working on resolving single atoms on the lattice sites.
K1.00246 Electronic and Magnetic Properties of B$_5$CX (X=V, Cr, Mn, Fe, Ni, and Co): a Theoretical Study, DAYNE SHIELDS, Department of Physics, University of Nebraska at Omaha, WAI-NING MEI, JING LU, Department of Physics, Peking University, PETER A. DOWBEN, Department of Physics, University of Nebraska at Omaha COLLABORATION, DEPARTMENT OF PHYSICS, PEKING UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA-LINCOLN COLLABORATION — We used on-site correlation corrected density functional theory to investigate the structure and magnetic properties of the recently synthesized B$_5$CX-Co and many other substitutions. We found that the Co and Ni molecules were non-magnetic. Other than that, Cr had both stable ferro- and antiferromagnetic structures. The V, Mn, and Fe molecules are not stable, we have to treat them as infinitely long chain molecules.

K1.00247 Scattering in Quantum Lattice Gases, ANDREW O’HARA, PETER LOVE, Haverford College — Quantum Lattice Gas Automata (QLGA) are of interest for their use in simulating quantum mechanics on both classical and quantum computers. QLGAs are an extension of classical Lattice Gas Automata where the constraint of unitary evolution is added. In the late 1990s, David A. Meyer as well as Bruce Boghosian and Washington Taylor produced similar models of QLGAs. We start by presenting a unified version of these models and study them from the point of view of the physics of wave-packet scattering. We show that the Meyer and Boghosian-Taylor models are actually the same basic model with slightly different parameterizations and limits. We then implement these models computationally using the Python programming language and show that QLGAs are able to replicate the analytic results of quantum mechanics (for example reflected and transmitted amplitudes for step potentials and the Klein paradox).

K1.00248 Novel approach to the dynamics of a dissipative two-state system, PETER P. ORTH, ADILET IMAMBIEKOV, KARYN LE HUR, Yale University — A two-state system in contact with a harmonic oscillator bath is frequently used to describe the process of decoherence in physical systems, such as a spin in a solid-state environment or a qubit coupled to external and uncontrolled degrees of freedom. The problem in general cannot be solved exactly, and several approximative methods have been devised such as Bloch-Redfield master equations, which are limited to weak-coupling, or the Non-Interacting Blip Approximation (NIBA), that neglects the system’s backaction onto the bath. We study the dissipative two-state dynamics in a novel way, rephrasing the problem as that of (non-)unitary time evolution of a quantum state vector exposed to a random Gaussian perturbation Hamiltonian. Our formalism goes beyond the NIBA and is particularly well suited to study the case of time-dependent system parameters. We compare it to common approaches such as the (extended)-NIBA, or stochastic wave-function methods. Furthermore, we investigate dissipative Landau-Zener tunneling in the so-called scaling limit.

K1.00249 Classical Derivation of Fermion Operators and Correlations, ROBERT CLOSE, None — A second-order wave equation is derived for an ideal elastic solid. The Klein-Gordon equation is a special case of this equation in which the mass term replaces the nonlinear rotation and convection terms. The second-order wave equation is factored to yield a first order bispinor equation. This equation is similar to the Dirac equation. The corresponding Lagrangian is constructed in terms of bispinors. The quantity conjugate to angular velocity is the quantum mechanical angular momentum. The quantity conjugate to velocity includes the quantum mechanical wave momentum and also the momentum of the medium. Along a given axis there are two independent solutions corresponding to forward- and backward-propagating waves. Since these independent states are separated by 180 degrees, their bispinor wave functions transform under rotation with spin one-half. Potentials are derived from consideration of wave interference. Parity is conserved. The conventional Dirac parity operator is incorrect because it represents a 180 degree rotation rather than inversion of velocity space. Correlations between classical bispinor wave functions are identical to the quantum correlations.

K1.00250 Modeling and Simulation of Fault Tolerant Quantum-dot Cellular Automata Devices, BENJAMIN PADGETT, Ball State University, GABRIEL ANDUWAN, Papua New Guinea University of Technology, MICHAEL KUNTZMAN, University of Texas, IOAN STURZU, Texas A&M University — We present a theoretical study of fault tolerant properties in Quantum-dot Cellular Automata (QCA) Devices. The study consists of modeling and simulation of various possible manufacturing, fabrication and operational defects. We will present specifically the effects of temperature and manufacturing defects at the cell level and array level of various QCA devices. Results of simple devices such as quantum wire, logical gates, inverter, cross-over and XOR will be presented. The cell defects would include displaced dots and missing defects. We will present specifically the effects of temperature and manufacturing defects at the cell level and array level of various QCA devices. Results of simple devices such as quantum wire, logical gates, inverter, cross-over and XOR will be presented. The cell defects would include displaced dots and missing defects.

K1.00251 Fault-Tolerant Characteristics of Quantum-dot Cellular Automata Devices, MAHUZA KHATUN, Ball State University, GABRIEL ANDUWAN, Papua New Guinea University of Technology, IOAN STURZU, Texas A&M University — The operational behavior of the Quantum-dot Cellular Automata (QCA) devices has been investigated regarding both dot displacement and temperature effects. Each of the breakdown characteristics displayed unique features for every particular QCA device. We have found that the characteristic features of the basic logic QCA devices are inherited by the higher or complicated QCA devices, such as the full adder. It was observed that the presence of a crossover of QCA lines in a full adder was a major factor for the breakdown. Thus, a proposed full adder QCA device without a crossover was seen to improve the successful operation of a full adder.

K1.00252 Extraction of correlated 2-photons with near unity efficiency, ALEXANDER LING, JUN CHEN, JINGYUN FAN, ALAN MIGDALL, JQI/NIST — We report a source of 2-photons that can be extracted with near unit efficiency. The reduced mode area of solid-core microstructure fibers lets a light pulse induce significant nonlinear optical interaction inside a short fiber, making it easy to generate 2-photon entanglement. However, the photon extraction efficiency is low due to the small core size ($d \approx 1 \mu m$) that requires high numerical aperture (NA) lenses to couple light in and out of the fiber. Tapering the core at the fiber end to 10 µm allows the use of anti-reflection-coated lenses of smaller NA, to achieve a single-photon extraction efficiency of $\eta = 96\%$. Using a pair of volume holographic gratings for selecting any wavelength of interest increased our spectral transmittance for that wavelength to $\eta_g = (98\%)^2$, enabling a near unit efficiency in extracting a single photon from the fiber source: $\eta \eta_g = 92.2\%$. The final 2-photon detection efficiency of 10% also extends the efficiency of single-photon detection modules (~70% each) and single-mode fiber collection (~50% per channel). At an average pump power of $P = 50 \mu W$ and a laser repetition rate of $R = 76$ MHz, we detect 50 photon pairs $s^{-1}$ with $g^{(2)}(0) = 0.0055$ and a coincidence-to-accidental ratio of 900:1. Higher pairs rates at the same $g^{(2)}$ level can be achieved by increasing R. With better photon detection, this source may enable loophole-free Bell tests.
K1.00253 Negativity for spin one anisotropic Heisenberg clusters in magnetic field, ARMEN KOCHARIAN, California State University, Los Angeles, NERSES ANANIKYAN, LEV ANANIKYAN, YAHAQN AGBARYAN, Yerevan Physics Institute — The quantum and thermal phase transitions are studied for spin $s=1$ in anisotropic (ferromagnetic and antiferromagnetic) XXZ and Heisenberg small clusters with longitudinal crystalline and magnetic fields. We investigate the concept of entanglement. The grand canonical ensemble of Heisenberg clusters is also used for exact analytical and numerical calculations of thermal properties and negativity as a function of magnetic and anisotropic fields. We study the negativity, magnetic phase transitions and crossovers in small clusters of various topologies driven by exchange interaction, external field and temperature. The negativity effect as a function of temperature and magnetic field is studied for both ferromagnetic and antiferromagnetic cases. The thermal behavior of negativity can capture the important properties in single molecule magnets, the dynamic magnetization and these our results can be useful for interpretation of the phase diagram in molecular nanomagnets and nanometer-sized magnetic particles.

K1.00254 Cavity -Quantum Dot interactions and mode coupling in a nanocavity, VIJAY KASIO-MAYAULJ, ONOFRIO RUSSO, New Jersey Institute of Technology — We describe an approach for realizing effective manipulation of single electron state level transitions for quantum dots mediated by a nano-cavity. The two quantum dots interact with the cavity for the two dot system in the coulomb blockade energy region. Because of the zero dimensional structure of the quantum dots, the system can be implemented to be a characteristic entity for an efficient generator of single photons. This process is emphatically more selective in the coulomb/spin blockade region, where also, the system efficiency of the single photon event is most likely more probable. Whereas, it is clear that the photon efficiency is small, the cavity quantum electrodynamics (CQED) nature suggests an enhancement in the electron energy state being occupied by the second quantum dot. This is more likely with very strong coupling of the quantum dots to the cavity with cavity quality factors larger than perhaps $10^5$. Quality factors in excess of $10^5$ have been demonstrated experimentally. 1. K. Srinivasan, M. Barselli, T. J. Johnson, P. E. Barclay, O. Painter, A. Stintz, and S. Krishna, Appl. Phys. Lett. 86, 151106 (2005). [ISI]

K1.00255 Linear, Rotational and Vibrational KInetic Energies Must Be Included in Mass-Energy Calculations, STEWART BREKKE, Northeastern Illinois University (former grad student) — All bodies have no motion, have linear, rotational and/or vibrational motion, singly or in some combination. Curvilinear motion is linear motion influenced by an external force field. The total energy of a body therefore must include the linear rotational and vibrational kinetic energies if present besides just the mass-energy conversion which may reconcile experimental data with theory even though these extra energies may be very small in comparison. If $k$ is a force constant, $x$ is the amplitude of vibration and $\omega$ is the angular speed, the formula for $E$ zero is as follows.

$$E_{0} = m\omega^{2} + 1/2m\omega^{2} + 1/2I\omega^{2} + 1/2kx^{2}$$

K1.00256 Consciousness Can Change the Output Signals of a Solar Cell and the Photoelectric Conversion Equation of Slow Mass Wave, DAYONG CAO, Beijing Natural Providence Science & Technology Development Co., LTD — The experiment's results show that human consciousness can change output signals such as $V_{oc}$ (open-circuit voltage) and $I_{sc}$ (short circuit current) of a solar cell placed some distance from a participant. For the first time, a consciousness signal is able to be recorded through the experiment conducted in Oct 2002. The order and rhythm of the changing wave pattern of $V_{oc}$ is related to the action of consciousness. The order and rhythm of slow brain signal of ERP and EEG are related to the cognized objects. Consciousness is independent and self-determined while brain signal is passive and driven. Consciousness is spiritual and Intelligence while brain signal is physical, corporality and mechanic. So consciousness is different from the brain signal. And consciousness effect is different from physical effect of light. Because consciousness can choose the object which it acts on. The light have a pair of mass wave of low frequency and energy wave of high frequency. In photoelectric conversion process, We only use the energy wave to get the $\eta$ (photoelectric transformation efficiency) which is little. If being used a pair of wave, we will get a larger $\eta$. The photoelectric conversion equation of slow mass wave are being put forward.

K1.00257 Quantum Quasi-Paradoxes and Quantum Sorites Paradoxes, FLORENTIN SMARANDACHE, University of New Mexico, Gallup Campus — There can be generated many paradoxes or quasi-paradoxes that may occur from the combination of quantum and non-quantum worlds in physics. Even the passage from the micro-cosmos to the macro-cosmos, and reciprocally, can generate unsolved questions or counter-intuitive ideas. We define a quasi-paradox as a statement which has a prima facie self-contradictory support or an explicit contradiction, but which is not completely proven as a paradox. We present here four elementary quantum quasi-paradoxes and their corresponding quantum Sorites paradoxes, which form a class of quantum quasi-paradoxes.

K1.00258 BIOLOGICAL PHYSICS —

K1.00259 Nonmonotonic Behavior of Nonnative Contacts in Small Proteins: An Exact Study on a Square Lattice, CHONG, CHEN, PURUSHOTTAM GUJRATI — Nonnative contacts are defined as contacts absent in the native state, and can be used to study the process of folding. They are expected to increase with temperature or energy. By exactly generating all possible conformations on a square lattice, we have investigated nonnative contacts for proteins in the standard HP model and its modified versions introduced by our group. This enables us to carry out exact calculation for the nonnative contact density $n_n(e)$ as a function of the energy density $e$ as well as its canonical average $\bar{n}_n(T)$ as a function of temperature $T$ from which we construct $\bar{n}_n(T)$ to compare with $n_n(e)$. The sequence dependence of $n_n(e)$ and $\bar{n}_n(T)$ are also investigated. Some new understandings of the role for nonnative contacts play in the protein folding process, as will be discussed during the talk. 1) The density $n_n(e)$ is always monotonically increasing in the standard model. This need not be true for all kinds of interactions. 2) The density $\bar{n}_n(T)$ is usually monotonically increasing. A few violations can be seen. 3) The protein property is sequence dependent, as expected. Reference [1] P. D. Gujrati, B. Lambeth, Jr., A. Corsi, and E. Askanazi, arXiv: 0708.3739 (2007).

K1.00260 Photoreceptor rearrangement and vision restoration in eyes with outer retinopathy: Quantitative assessment by fractal analysis, DELIA CABRERA DEBUC, Bascom Palmer Eye Institute, University of Miami Miller School of Medicine, ROBERT TCHTINGA, University of Dschang, Faculty of Science, Department of Physics, P.O.Box 67 Dschang, Cameroon, MEDICAL IMAGING COLLABORATION, FRACTAL ANALYSIS COLLABORATION — The differentiation between normal and abnormal photoreceptor rearrangement with outer retinopathy before and after treatment may improve understanding on the sequence of events involved in the visual field defects. In this study, we evaluated a fractal analysis approach to quantify photoreceptor rearrangement and vision restoration. We analyzed Optical Coherence Tomography (OCT) data from an individual with outer retinopathy before and after treatment. The outer nuclear layer (ONL) was delineated from the rest of the retinal structure by using a custom-built segmentation algorithm. We then determined the fractal box dimension of the ONL's outline using the box counting method. Thickness and reflectance of the ONL were also calculated. Our results showed that the ONL's fractal dimension, thickness and relative reflectivity decreased after treatment. These early results showed that ONL's fractal dimension could be used as an index of photoreceptor rearrangement, which might lead to a more effective approach to therapy and improved diagnosis.
**K1.00261 Statistical Characterization of a 1D Random Potential Problem— with applications in score statistics of MS-based peptide sequencing**

GELIO ALVES, YI-KUO YU, National Center for Biotechnology Information/NIH — We provide a complete thermodynamic solution of a 1D hopping model in the presence of a random potential by obtaining the density of states. Since the partition function is related to the density of states by a Laplace transform, the density of states determines completely the thermodynamic behavior of the system. We have also shown that the transfer matrix technique, or the so-called dynamic programming, used to obtain the density of states in the 1D hopping model may be generalized to tackle a long-standing problem in statistical significance assessment for one of the most important proteomic tasks--peptide sequencing using tandem mass spectrometry data.

This work was supported by the Intramural Research Program of the National Library of Medicine at the National Institutes of Health.

**K1.00262 ABSTRACT WITHDRAWN**

**K1.00263 Single Molecule Study on Incorporation Efficiency of DPO4 and Klenow Fragment to BPDE Adduct**

LU SONG, UC Davis, LLNL, YIN YEH, ROD BALHORN, MONIQUE COSMAN, UC Davis — DNA synthesis involving high fidelity A-family polymerases such as Klenow fragment is blocked by DNA adducts, while Y-family DNA polymerases such as Dpo4 can bypass the DNA adducts to resume DNA synthesis. So understanding the functional relationship between A-family and Y-family DNA polymerases in DNA replication and the mechanism of bypassing DNA adducts is of great help to explain the cause of mutagenesis. We introduce a flow cell on modified surface to study the incorporation efficiency of Dpo4 and Klenow fragments to benzo[α]pyrene-diol-epoxide (BPDE) adduct at single molecule level. Specifically, we anchor the labeled DNA onto the modified surface with adduct site open in nucleotide incorporation and flow the polymerases and labeled nucleotides into flow cell. With Total Internal Reflection Fluorescence Microscopy (TIRFM) we identify the incorporation of the nucleotides onto the anchored DNA template by identifying the co-localization of the template position and that of the labeled nucleotide. We further quantify the signal densities of the images obtained from the two different polymerases, thus examining whether incorporation reactions have been executed and quantifying the incorporation efficiency of the polymerases. We can also identify, on the specific adduct site, which nucleotide, if any, is incorporated by each of the two polymerases.

**K1.00264 Mechanical Properties of Type IV Pili in *P. Aeruginosa***

SHUN LU, AHMED TouHAMI, University of Guelph, EDIE SCHEURWATER, HANJEOng HARVEY, LORI BURROWS, McMaster University, JOHN DUTCHER, University of Guelph — Type IV pili (Tfp) are thin flexible protein filaments that extend from the cell membrane of bacteria such as *Pseudomonas aeruginosa* and *Neisseria gonorrhoeae*. The mechanical properties of Tfp are of great importance since they allow bacteria to interact with and colonize various surfaces. In the present study, we have used atomic force microscopy (AFM) for both imaging and pulling on Tfp from *P. aeruginosa* (PAO1) and from its PilA, PiIIT, and PiIc mutants. A single pilus filament was mechanically stretched and the resulting force-extension profiles were fitted using the worm-like-chain (WLC) model. The statistical distributions obtained for contour length, persistence length, and number of pili per bacteria pole, were used to evaluate the mechanical properties of a single pilus and the biogenesis functions of different proteins (PilA, PilIT) involved in its assembly and disassembly. Importantly, the persistence length value of ~ 1 µm measured in the present study, which is consistent with the curvature of the pilus observed in our AFM images, is significantly lower than the value of 5 µm reported earlier by Skerker et al. (1). Our results shed new light on the role of mechanical forces that mediate bacteria-surface interactions and biofilm formation. 1- J.M. Skerker and H.C. Berg, Proc. Natl. Acad. Sci. USA, 98, 6901-6904 (2001).

**K1.00265 Inhibition of Oncogenic functionality of STAT3 Protein by Membrane Anchoring**

BAOXU LIU, STEVEN FLETCHER, PATRICK GUNNING, CLAUDIU GRADINARU, University of Toronto, GRADINARU/GUNNING COLLABORATION — Signal Transducer and Activator of Transcription 3 (STAT3) protein plays an important role in oncogenic processes. A novel molecular therapeutic approach to inhibit the oncogenic functionality of STAT3 is to design a prenylated small peptide sequence which could sequester STAT3 to the plasma membrane. We have also developed a novel fluorescence derivative label (F-NAC), which is much more photostable compared to the popular fluorescein label FITC. Remarkably, the new dye shows fluorescent properties that are invariant over a wide pH range, which is advantageous for our application. We have shown that F-NAC is suitable for single-molecule measurements and its properties are not affected by ligation to biomolecules. The membrane localization via high-affinity prenylated small-molecule binding agents is studied by encapsulating F-NAC-labeled STAT3 and inhibitors within a liposome model cell system. The dynamics of the interaction between the protein and the prenylated ligands is investigated at single molecule level. The efficiency and stability of the STAT3 anchoring in lipid membranes are addressed via quantitative confocal imaging and single-molecule spectroscopy using a custom-built multiparameter fluorescence microscope.

**K1.00266 Towards real-time 3D Tracking of Structural Transitions in Adenylate Kinase by Thermal Noise Imaging**

ARND PRAALLE, VIJAY RANA, YUNSHIANG HSU, University at Buffalo, SUNY — Proteins in contrast to macroscopic machines are subject to thermal fluctuations in shape which provide both opportunities and challenges. They have to be flexible enough to support turn-over rates up to hundreds per second, yet stable enough to maintain their three-dimensional structure over hours and days. As result of thermal excitation they fluctuate between structural conformations. We measured thermally excited structural fluctuations in the Adenylate Kinase using a site-specifically attached nanoparticle and a laser trap based position sensing scheme. This ‘Thermal Noise Imaging’ (TNI) can provide real-time tracking of 3D structural transitions. TNI uses scattering of laser light to locate a nanoparticle with Ångström spatial and microsecond temporal resolution. We present details of the technique and a comparison of thermally excited structure fluctuations with functional transitions.

**K1.00267 Single molecule study of ClpP enzymatic activity**

AMIR MAZOUCHi, University of Toronto, Department of Physics, ANGELA YU, WALID HOURY, University of Toronto, Department of Biochemistry, CLAUDIU GRADINARU, University of Toronto, Department of Physics, GRADINARU TEAM, HOURY TEAM — Elementary processes that form the basis of biological activities pass through a number of short-lived intermediate states while progressing from initial state to final state. Single-molecule techniques, unlike ensemble averaging measurements, are often able to resolve these transient states. ClpP, a known target of antibacterial drugs like acycepidopes (AEDPs), is a classical representative of serine proteases, enzymes that cleave peptide bonds in proteins. We performed single-molecule fluorescence measurements including burst spectroscopy and fluorescence correlation spectroscopy (FCS) to address unknown aspects of this degradation process. Our study reveals important molecular details of protein degradation, such as the enzyme-substrate binding rate, the lifetime distribution of the conjugated state and the probability of substrate cleavage upon conjugation.
K1.00268 The effect of macromolecular crowding on reaction rates: a computational and theoretical study1, JUN SOO KIM, ARUN YETHIRAJ, Theoretical Chemistry Institute and Department of Chemistry, University of Wisconsin-Madison — The effect of macromolecular crowding on the rates of association reactions was investigated using theory and computer simulations. Reactants and crowding agents are both hard spheres, and when two reactants collide they form product with a reaction probability, \( p_{\text{reac}} \). A value of \( p_{\text{reac}} < 1 \) crudely mimics the fact that proteins must be oriented properly in order for an association reaction to occur. The simulations show that the dependence of the reaction rate on the volume fraction of crowding agents varies with the reaction probability. For reaction probabilities close to unity where most of encounters between reactants lead to a reaction, the reaction rate always decreases as the volume fraction of crowding agents is increased due to the reduced diffusion coefficient of reactants. On the other hand, for very small reaction probabilities where in most of encounters the reaction does not occur, the reaction rate increases with the volume fraction of crowing agents, in this case, due to the increase probability of a re-collision. The Smoluchowski theory is in quantitative agreement with simulations for the reaction rate constant and allows the quantitative analysis of both effects separately.

1Supported by the National Science Foundation under Grant No. CHE-0717569.

K1.00269 Polymer translocation induced by bad solvent, CHRISTOPHER LORSCHER, ANIKET BHATTACHARYA, University of Central Florida, TAPIO ALA-NISSILA, Helsinki University of Technology — We report Langevin dynamics simulation studies of a translocating homopolymer through a nano pore induced by different existing solvent conditions at the cis and trans compartments of the pore. Specifically, we study the mean first passage time \( \tau \) as a function of the chain length \( N \) and determine the scaling exponent \( \alpha \sim N^{-\alpha} \). We also look at the mean force experienced by the chain and its conformations as a function of the translocated segments. Our studies also reveal detail picture of the translocation process which may provide insights relevant for the entry of a DNA into a host cell.

K1.00270 Statistical test of a null hypothesis: Taser® shocks have not caused or contributed to subsequent in-custody deaths, MARJORIE LUNDQUIST1, Bioelectromagnetic Hygiene Institute — Since 1999 over 425 in-custody deaths have occurred in the USA after law enforcement officers (LEOs) used an M26 or X26 Taser®, causing Amnesty International and the ACLU to call for a moratorium on Taser use until its physiological effects on people have been better studied. A person’s Taser dose is defined as the total duration (in seconds) of all Taser shocks received by that person during a given incident. Utilizing the concept of Taser dose for these deaths, TASER International’s claim of Taser safety can be treated as a null hypothesis and its validity scientifically tested. It shows that the null hypothesis should be rejected; i.e., model M26 and X26 Taser®s are capable of producing lethal effects non-electrically and so have played a causal or contributory role in a great many of the in-custody deaths following their use. This implies that the Taser® is a lethal weapon, and that LEOs have not been adequately trained in its safe use!

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K1.00271 Computing Transitions in Macromolecular Systems: Dynamic Importance Sampling, JUAN PERILLA, Johns Hopkins University, OLIVER BECKSTEIN, ANU NAGARAJAN, THOMAS WOOLF — Understanding and predicting conformational changes in macromolecules is central to linking structure and function. Performing straight-forward all-atom molecular dynamics would, in principle, enable sampling of conformational changes, but the time-scale for functionally important transitions, exceeds the usual MD timescales by several orders of magnitude. Thus to sample on longer time-scales requires the development of biased molecular dynamic methods, where the bias can be applied and corrected for at the end. In our approach, called ‘Dynamic Importance Sampling’ we generate a series of independent trajectories that are conditioned on starting and ending in defined conformations. Trajectories are generated using two different algorithms: one that uses an adaptive soft-ratcheting scheme, based on stochastic trajectories and, the other uses information from the set of normal modes. Both algorithms do not require a previous knowledge on the reaction coordinate, furthermore using this framework we are also able to introduce a generalized reaction coordinate in order to guide the transitions for virtually any system. The algorithms, which require no initial pathway, are capable of rapidly determining multiple pathways between known states. The associated probability scores allow us to rank order the most likely pathways.

K1.00272 The Origin of Power Law Distributions in Protein Synthesis, JEFFREY BARKER, CHUCK YEUNG, Pennsylvania State Univ. at Erie, XIAO-LUN WU, EMILY CHAPMAN-MCUYSTON, University of Pittsburgh — A genetically identical bacteria population will show heterogeneous gene expression due to the stochastic nature of the protein production mechanism. Therefore, the probability distribution of the resulting protein(s) can be used to gain information about these underlying processes. The experiments of Chapman-McQuiston et. al. show that under certain circumstances the protein probability distribution has a power law form \( p(n) \sim n^{-\alpha} \) at small \( n \). Our simulations and analysis find, in agreement with work by Friedlander and Brenner, that a linear protein production rate will produce a power law distribution with the exponent depending on the amplitude of the bubble (bubble) dynamics of 80 bp long promoter DNA sequences. We suggest that three dynamic quantities: bubble probability, bubble lifetime, and average strand is likely to be a requirement for transcription initiation in several promoters. We present molecular dynamic simulations of DNA to analyze the strand separation site.

K1.00273 Toward a Detailed Description of the Thermally Induced Dynamics of the Core Promoter, BOIAN ALEXANDROV, Theoretical Division, Los Alamos National Laboratory, VLADIMIR GELEV, Beth Israel Deaconess Medical Center and Harvard Medical School, KIM RASMUSSEN, ALAN BISHOP, Theoretical Division, Los Alamos National Laboratory, ANNY USHEVA, Beth Israel Deaconess Medical Center and Harvard Medical School — Experimental data suggest that a spontaneous dsDNA strand separation at the transcriptional start site (TSS) is likely to be a requirement for transcription initiation in several promoters. We present molecular dynamic simulations of DNA to analyze the strand separation (bubble) dynamics of 80 bp long promoter DNA sequences. We suggest that three dynamic quantities: bubble probability, bubble lifetime, and average strand separation, together represent an adequate characterization of the bubble formation at TSS’s of eight mammalian gene promoters. The TSS is distinguished by large, frequent, and long-lived transient openings in the double helix. In support of these results are our experimental transcription data demonstrating that an artificial DNA template, viz., a bubble-template of 5 bp mismatch at the TSS, is transcribed bi-directionally by human RNA polymerase alone in the absence of any other transcription factors.

K1.00274 In Silico Docking of Ligands to Drug Oxidation Enzymes Cytochrome P450 3A4 and Cytochrome P450 1A2, DAVID SMITH, JONATHAN GUGLIELMONE, MARSCH GLENN, GUENGERICH F. PETER, GROVE CITY COLLEGE BIOPHYSICS RESEARCH TEAM — Cytochrome P450 3A4 (CYP3A4) and Cytochrome P450 1A2 (CYP1A2) oxidize most drugs in humans. Protein modeling toolkits from OpenEye Scientific Software were used to examine the interaction of drug substrates with CYP3A4 and CYP1A2. Conformers and partial atomic charges were generated for each drug molecule. User-defined volumes were defined around CYP3A4 and CYP1A2 active sites. Ligands were docked assuming protein and substrates as rigid bodies. To assess rigid docking accuracy, x-ray diffraction coordinates of CYP3A4-erythromycin and CYP3A4-metyrapone complexes were obtained. Rigid re-docking of erythromycin and metyrapone into CYP3A4 yielded poses similar to the crystal structures. Rigid docking revealed two other energetically-favorable CYP3A4-metyrapone poses. The best poses were obtained by using all the Open Eye scoring functions. Optimization of protein-ligand interactions within 5-10 Angstroms of the docked ligand was then performed using the Merck Molecular Force Field in which the protein was assumed to be flexible and the ligand to be rigid. Nearby protein residues pulled slightly closer to the substrate, reducing the volume of the active site.
K1.00275 Examination of mathematical models for voltage attenuation in dendritic trees of geniculate neurons, KEEGAN HINES, Washington and Lee University, WILLIAM GUIDO, Virginia Commonwealth University — An examination of Rall’s model of Electrotonic Compactness in neuronal dendritic trees was conducted. The principal power of this model is a prediction for dendritic morphology as it is related to voltage attenuation and efficient transmission of electrical signals. In particular, this study tested the validity of Rall’s “3/2 power rule” with precision and accuracy not previously sought. Cells were imaged using fluorescent tagging and multi-photon confocal microscopy in order to render three dimensional images of cells in vivo. Dendritic diameters and lengths were measured on either side of junction points and these values were compared to Rall’s predictions. Cells of varying ages were measured in order to simultaneously investigate whether deviations from Rall’s model increased or decreased with brain development. Cells of age P8 tend to adhere closely to Rall’s predictions while mature cells (∼P90) show morphologies which would lead to inefficient signal flow. These data coincide well with previous studies which indicate that as cells grow, membranes mature and acquire ion channels which lead to non-linear conductances across the membrane. This is a possible explanation for why, from a purely morphological standpoint, cells grow into a less electrically efficient formation.

K1.00276 The Interaction of Photon Beams with the DNA Molecules: Genomic Medical Physics, V. ALEXANDER STEFAN, Institute for Advanced Physics Studies (Stefan University), 1010 Pearl Street, La Jolla, CA 92038-2946 — I propose a novel method for the modification of the corrupted human DNA code that causes particular genetic disease. The method is based on the nonlinear interaction between the DNA molecule and the “modulation photons” generated by the BW-FEL. The BW-FEL frequencies are given by ε=ω−2γΩe(γ is the free electron beam relativistic factor, n is the harmonic number of the electron Bernstein plasma mode, and Ωe is the electron cyclotron frequency). The “carrier photons” are focused on the area of the brain, the source-center of a genetic disease. For the BW-FEL parameters: the free electron beam guiding d.c. magnetic field ~ 1kG, γ ~10^3, and n=10, the keV “modulation photons” are generated, which are easily focused on the nucleotides. By modulating the frequency of the BW-FEL, the parametric resonance with the different DNA (sub-DNA) eigen molecular oscillation-modes are achieved, leading to the “knock-on” of the unwanted (corrupted) nucleotides.

K1.00277 A kinetics study of the activation energy for the desorption of water from guanosine, MEGAN SCHWENKER SMITH, SCOTT LEE, University of Toledo — The interactions of the nucleic acids with their water of hydration are of fundamental importance but are still poorly characterized. As an initial effort, we have studied the nucleoside guanosine (G), composed of the ribose sugar and the guanine base, which is a component of RNA. We have measured the interactions of the water of primary hydration with G via thermogravimetric measurements and differential thermal analysis by studying the kinetics of the dehydration process. These data yield the activation energy for the desorption of the water of primary hydration from G.

K1.00278 Novel techniques for study of the nucleosome core particle ionic atmosphere and its role in electrostatically-driven DNA packing, KURT ANDRESEN, Colgate University — The nucleosome core particle (NCP) is the primary mechanism for DNA compaction. While the wrapping of the DNA around the histone core is thought to be at least partially sequence-dependent, the packing of the nucleosome cores is believed to be almost entirely electrostatic in nature. Using novel techniques to probe the ionic atmosphere, we hope to elucidate details of this compaction and provide a quantitative description of the positive and negative ions that surround the nucleosome. Results of these experiments will be presented. This work should have implications for nucleosome compaction, chromatin remodeling, and more generally electrostatics of highly charged biomolecules.

K1.00279 Hill Parameters and Heterogeneity of alpha-Naphthoflavone Binding to Human Cytochrome P450 3A4 by Fluorescence Spectroscopic Analysis, BENJAMIN CARLSON, GLENN MARSCH, Grove City College, MARTHA MARTIN, P. F. BEER GUENGERICH, Vanderbilt University School of Medicine — Human cytochrome P450 3A4 (CYP 3A4) is an alpha-helical membrane-bound protein that metabolizes approximately 50% of all drugs. The interaction between CYP450 3A4 and alpha-naphthoflavone (ANF) was characterized using fluorescence methods. ANF quenched fluorescence from tryptophan residues in CYP 3A4, and CYP 3A4 quenched bound ANF. The ANF emission energy was unchanged upon binding to CYP 3A4, implying that enzyme-bound 3A4 is completely quenched. Fluorescence difference spectra were fit to the Hill equation by varying the parameters Kd and n. For quenching of tryptophan fluorescence by ANF, no significant sigmoidal behavior was observed with n=1.1, and the spectral dissociation constant revealed a strong ANF-CYP 3A4 interaction with Kd=27nM. Modest cooperativity and very tight binding was observed in the quenching of ANF by CYP 3A4, with n=1.4 and Kd=4.9nM. Fluorescence polarization anisotropy decreased at low ANF/CYP 3A4 molar ratios; then < r > increased at higher ratios. Compared to substrate-free CYP 3A4, adding substrate at low molar ratios increases the CYP 3A4 rotation, suggesting the molecular volume decreases.

K1.00280 Residue mobility and energy profiles of an HIV-1 protease (1DIFA) chain by a coarse-grained Monte Carlo simulation, RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — HIV-1 protease (1DIFA), an enzyme consists of two polypeptides, 99 amino acids each. Aspartic acid residue (Asp) forms the active catalytic site. Specificities of residues are captured via an interaction matrix (residue-residue, residue-solvent) of the Lennard-Jones potential. Simulations are performed for a range of interaction strength (J) with the solvent-residue interaction describing the quality of the solvent. Snapshots of the protein show considerable changes in the conformation of the protein on varying the interaction. From the mobility and energy profiles of the residues, it is possible to identify the active (and not so active) segments of the protein and consequently their role in proteolysis. Contrary to interaction thermodynamics, the hydrophobic residues possess higher configurational energy and lower mobility while the electrostatic and polar residues are more mobile despite their lower interaction energy.

K1.00281 Interaction of Human Cytochrome P450 3A4 with Hydrophobicity Probe Nile Red Shows Heterogeneous, Strong Binding, JENNIFER HANSEN, F. GUENGERICH, MARTHA MARTIN, GLENN MARSCH, PHYSICS DEPARTMENT, GROVE CITY COLLEGE, GROVE CITY PA 16127 TEAM, CENTER IN MOLECULAR TOXICOLOGY, VANDERBILT UNIVERSITY, NASHVILLE, TN, 37232 TEAM — Human cytochrome P450 3A4 (CYP 3A4) binds an unusually wide variety of substrates, and metabolizes about 50% of all drugs. Steady-state fluorescence spectra were acquired for complexes of CYP 3A4 and the fluorescence probe Nile Red. Difference fluorescence spectra showed the quenching of CYP 3A4 tryptophan fluorescence by Nile Red. CYP 3A4 was also added to Nile Red, and changes in the Nile Red fluorescence spectra were monitored. The dissociation constant showed tight binding, with Kd = 44nM. Good fits to the Hill plots were obtained with n = 1, suggesting non-cooperative binding. This study revealed strong, heterogeneous, non-cooperative binding of Nile Red to CYP 3A4.
The Effect of Electric and Magnetic Fields on Protein Self-Organization and Osteoblast Biomineralization

The Effect of Titanium Dioxide Nanoparticles on Keratinocyte Cell (KC) and Squamous Cell Carcinoma (SCC) - Investigation on mineralization behaviour of Type I collagen and noncollagenous extracellular matrix protein immobilized on polymer thin film. XIAOLAN BA, Stony Brook University, ARIELLA KRISTAL, Solomon Schechter Highschool, ELAINE DIMISI, Brookhaven National Laboratory, MIRIAM RAFAILOVICH, Stony Brook University — The effects of the components of extracellular matrix on the bone formation and the kinetics of crystal growth of calcium phosphate have remained unknown. Here we reported a method to investigate the role of Type I collagen and the interactions with other ECM proteins such as fibronectin and elastin during biomineralization process. The early stage of mineralization was characterized by atomic force microscopy (AFM) and shear modulation force microscopy (SMFM). The late stage of mineralization was investigated by scanning electron microscopy (SEM), grazing incident x-ray diffraction (GIXD). The results showed the calcium phosphate biomineralization only occurred when the collagen interacted with fibronectin or elastin.

K1.00283 Effects of cholesterol and unsaturated DOPC lipid on chain packing of saturated gel-phase DPPC bilayers

K1.00284 Motional Coherence in Fluid Phospholipid Membranes

K1.00285 Coarse-grain Modeling of Lipid Membrane Adsorption on Nanopatterned Surfaces

The Effect of cholesterol and unsaturated DOPC lipid on chain packing of saturated gel-phase DPPC bilayers

K1.00286 The Effect of Titanium Dioxide Nanoparticles on Keratinocyte Cell (KC) and Squamous Cell Carcinoma (SCC-13)

K1.00287 Theoretical Description of Microtubule Dynamics in Fission Yeast During Interphase

K1.00288 The Effect of Electric and Magnetic Fields on Protein Self-Organization and Osteoblast Biomineralization

Coarse-graining of the membrane lipids and surface allow for the larger system size necessary for membrane shape studies. Supported lipid bilayers (SLB) continue to be an important means of measuring the thermodynamic and mechanical properties of phospholipid membranes, which are the basis of compartmentalization in living cells. Understanding SLB systems with respect to their substrates enhances the understanding of the measurements taken thereon and promotes design of new substrates to expand the usefulness of these systems. We present data for the interaction of coarse-grained lipid membranes with nanopatterned surfaces, showing the effect of the balance between bending energy and adsorption energy on membrane topology.

The Effect of Titanium Dioxide Nanoparticles on Keratinocyte Cell (KC) and Squamous Cell Carcinoma (SCC) cells. Confocal microscope shows that the particles in keratinocyte culture are sequestered in membranes between the cell colonies. The particles penetrated into the cells in the case of the SCC cells. TEM revealed very few particles in the keratinocyte, many more particles were observed sequestered in vacuole of the SCC cells. These results indicate that the keratinocyte layer behaves very different from the fibroblast layers which are much more senescent to TiO₂ nanoparticle damage and may suggest a protection mechanism of the dermal tissue. The effect of UV exposure in the presence of DNA was also investigated. We found that adsorbed proteins, as well as grafted polymer provided a measure of protection against free radical formation. The effects of low level UV exposure when the particles are near in-vitro cell culture will be presented.

Substrate interactions with adsorbed membranes modify the intrinsic mechanics of supported lipid bilayers. Coarse-graining of the membrane lipids and surface allow for the larger system size necessary for membrane shape studies. Supported lipid bilayers (SLB) continue to be an important means of measuring the thermodynamic and mechanical properties of phospholipid membranes, which are the basis of compartmentalization in living cells. Understanding SLB systems with respect to their substrates enhances the understanding of the measurements taken thereon and promotes design of new substrates to expand the usefulness of these systems. We present data for the interaction of coarse-grained lipid membranes with nanopatterned surfaces, showing the effect of the balance between bending energy and adsorption energy on membrane topology.

The Effect of Titanium Dioxide Nanoparticles on Keratinocyte Cell (KC) and Squamous Cell Carcinoma (SCC-13) - CHIENHSIU LIN, SUNY-Stony Brook U., MARCIA SIMON, VLADIMIR JURUKOVSKI, WILSON LEE, MIRIAM RAFAILOVICH, DEPARTMENT OF MATERIALS SCIENCE & ENGINEERING, STONY BROOK UNIVERSITY, STONY BROOK, NEW YORK COLLABORATION — We have investigated the effects of TiO₂ nanoparticles on cell keratinocytes and SCC (Squamous Cell Carcinoma) cells. We found that the concentration of particles required to adversely affect the cells was many times higher for keratinocytes than SCC cells. Confocal microscope shows that the particles in keratinocyte culture are sequestered in membranes between the cell colonies. The particles penetrated into the cells in the case of the SCC cells. TEM revealed very few particles in the keratinocyte, many more particles were observed sequestered in vacuole of the SCC cells. These results indicate that the keratinocyte layer behaves very different from the fibroblast layers which are much more senescent to TiO₂ nanoparticle damage and may suggest a protection mechanism of the dermal tissue. The effect of UV exposure in the presence of DNA was also investigated. We found that adsorbed proteins, as well as grafted polymer provided a measure of protection against free radical formation. The effects of low level UV exposure when the particles are near in-vitro cell culture will be presented.

Theoretical Description of Microtubule Dynamics in Fission Yeast During Interphase - YUNG-CHIN OEI, ANDREA JIMÉNEZ-DALMARONI, University College London, UK, ANDREJ VILFAN, Jozef Stefan Institute, Ljubljana, Slovenia, THOMAS DUKE, University College London, UK — Fission yeast (S. pombe) is a unicellular organism with a characteristic cylindrical shape. Cell growth during interphase is strongly influenced by microtubule self-organization - a process that is experimentally well characterized. The microtubules are organized in 3 to 4 bundles, called “interphase microtubule assemblies” (IMAs). Each IMA is composed of several microtubules, arranged with their dynamic “plus” ends facing each other. Coarse-graining of the membrane lipids and surface allow for the larger system size necessary for membrane shape studies. Supported lipid bilayers (SLB) continue to be an important means of measuring the thermodynamic and mechanical properties of phospholipid membranes, which are the basis of compartmentalization in living cells. Understanding SLB systems with respect to their substrates enhances the understanding of the measurements taken thereon and promotes design of new substrates to expand the usefulness of these systems. We present data for the interaction of coarse-grained lipid membranes with nanopatterned surfaces, showing the effect of the balance between bending energy and adsorption energy on membrane topology.

The Effect of Electric and Magnetic Fields on Protein Self-Organization and Osteoblast Biomineralization - XIAOLAN BA, Stony Brook University, LARA FOURMAN, Plainview Old Bethpage Highschool, SANCITA SINGAL, Herricks Highschool, YIZHI MENG, MIRIAM RAFAILOVICH, Stony Brook University — The induction of bone formation to an intentional orientation is a potentially viable clinical treatment for bone regeneration. Among the many chemical and physical factors, electric and magnetic fields are an essential way to regulate the behavior of cells and matrix fibers. The aims of this study are to investigate the effects of electric and magnetic fields on protein self-organization and osteoblast biomineralization on polymer surfaces in vitro. To this end, we use atomic force microscopy (AFM) to characterize the morphology of protein fiber and ECM by cells. The mechanical property of protein fibers was investigated by shear modulation force microscopy (SMFM). The late-stage of mineralization was characterized by scanning electron microscopy (SEM) and grazing incident x-ray diffraction (GIXD). The primary data indicated that the magnetic field could enhance the biomineralization of osteoblast.
K1.00289 Elastic properties of vimentin networks1, YI-CHIA LIN, AMY C. ROWAT, Harvard University, HARALD HERRMANN, German Cancer Research Center, CHASE C. BROEDERSZ, FREDERICK C. MACKINTOSH, Vrije Universiteit, ELEONAR A. MILLMAN, DAVID A. WEITZ, Harvard University — We measure the mechanical properties of in vitro networks of the intermediate filament protein vimentin by rheometry. Vimentin networks are highly elastic even for small volume fractions of protein and exhibit dramatic stiffening with strain. We find that divalent ions such as Ca2+ and Mg2+ act as effective cross-linkers in the vimentin network. The observed linear and nonlinear elastic responses at intermediate strains can be explained quantitatively by affinely stretching the entropic fluctuations of single semiflexible filaments; at high strains, enthalpic stretching of the individual filaments contributes to the observed nonlinear response.

1This work was supported by the NSF (DMR-0602684 and CTS-0505929) and the Harvard MRSEC (DMR-0213805).

K1.00290 In Vitro Migration of Human Dermal Fibroblasts on the Electrospun Fibrous Scaffold, YING LIU, DILIP GERSASPE, ALICIA FRANCO, Stony Brook University, SARAJANE GROSS, ELIAS GOODMAN, North Shore Hebrew Academy High School, RICHARD CLARK, MIRIAM RAFAILOVICH, Stony Brook University — Cell migration has become the focus of much research due to its importance through out cell life. We hypothesized that the aligned scaffold obtained from electrospinning would enhance the rate of cell migration and ultimately the rate of new tissue ingrowth. An in vitro en-masse assay was used to study the effects of fiber diameter and alignment on the cell migration. It was found that, while the cells were spreading out on the fibers with diameter of 200nm, nearly all the cells were oriented along the fibers for the 1 and 8 micron surfaces. In addition to fiber diameter, orientation is another crucial parameter which can determine cell migration. Cell migration rates and persistence increased on the aligned PMMA fibers compared to the random fibers. The role of focal adhesions during cell migration was detected by staining the Vinculin after 6 and 24h of cell culture time. The computational model used to stimulate cell migration on the aligned scaffold, and it was turned out that various cellular parameter were integrated to accomplish the specific cell locomotion pattern on the aligned scaffold.

K1.00291 Nanoscale Mechanics of Type I Collagen, H. HARPER, E. CROPPER1, A. BULGER, U. CHOKSI, T. J. KOOB, S. PANDIT, W.G. MATTHEWS, University of South Florida — Collagen is the most abundant protein in the body by mass. Type I collagen fibrils provide mechanical strength and cellular housing within tissues exhibiting a broad range of mechanical properties. This diversity in the mechanics of tissues with similar underlying components warrants detailed study of the process by which structure and mechanics develop. While collagen mechanics have been studied at the tissue level for decades, surprising little is known about collagen mechanics at the fibril and molecular level. Presented herein is a multi-scale experimental and computational investigation of collagen I mechanics, bridging the single molecule and fibril hierarchical forms. The mechanics of single collagen molecules are explored using AFM and force spectroscopy. Moreover, atomistic molecular-dynamics simulations are performed to provide structural information not accessible to the experimental system. Fibrils then are grown from molecular collagen, and the mechanics of these fibrils are investigated using AFM. Based upon the single molecule and fibril results, a coarse-grain computational model is being developed. The outcomes include a better understanding of how the mechanics of filamentous self-organizing systems are derived and how their hierarchical forms are established.

1Co first author

K1.00292 Self-assembly of FKE8 peptides using CHARMM, ABBDELHALLAH OUAZZANI, ABDULKADER KARA, ANIKET BHATTACHARYA, University of Central Florida — We investigate the molecular self-assembly of FKE8 peptides (with a sequence FKFEFKFE) using CHARMM. Previous studies1,2 of the FKE8 peptides have shown helical ribbon structures during the formation of β-sheets. In order to understand this supramolecular structure, first we investigate the stable configuration of two FKE8 molecules as a function of the orientation of the long axis of the molecules. We find that stable configuration of these two molecules (based on energy minimization) occurs when the long axes of the two molecules are orientated at an angle ≃ 51.5° with respect to each other. This angle may be relevant to understand the pitch of the helical structure. Next we study the self-assembly of several FKE8 molecules starting with an initial configuration where two successive FKE8 molecules are oriented at an angle ≃ 51.5° with respect to each other. It was found that, while the cells were spreading out on the fibers with diameter of 200nm, nearly all the cells were oriented along the fibers for the 1 and 8 micron surfaces.


K1.00293 Simulation of Peptide Binding to Silica and Silica Mineralization, F.S. EMAMI, H. HEINZ, Department of Polymer Engineering, The University of Akron, Akron, Ohio, 44325, USA, R.J. BERRY, V. VARSHNEY, B.L. FARMER, R.R. NAIK, AFRL/RXB, WPAFB, Dayton, OH 45433, USA, S.V. PATWARDHAN, C.C. PERRY, Department of Chemistry, Nottingham Trent University, Nottingham, NG11 8NS, U.K. — The purpose of this study is to identify the nature of the interaction of peptides with silica surfaces and their effect on mineralization. Classical force fields (CVFF, PCFF) have been extended for silica aiming at the computation of surface properties in quantitative agreement with experiment, taking explicitly into account water molecules, pH, and surface coverage with peptides. We focus on the interaction of five short peptides (pep1, pep4, 82-4, H4, R5) identified by biopanning with regular and amorphous silica surfaces (Q3 and Q2) to understand the relation between peptide sequence and affinity to the surface. Results of the atomistic molecular dynamics simulation indicate adsorption energies, binding constants and conformational changes upon adsorption. The comparison of NMR chemical shifts in solution and on the surface in computation and experiment further aids in understanding the mechanism of binding.

K1.00294 NMR Studies in Macromolecular Solutions1, ANAND YETHIRAJ, SULIMAN BARHOUUM, Memorial University — We use diffusion nmr to characterize the dynamics of multi-component macromolecular solutions. Diffusion coefficients of all components are obtained simultaneously. We also present a scheme to extract the diffusion coefficients associated with transient aggregates in solution. Applications and limitations of this scheme are discussed.

1This work is being supported by NSERC

K1.00295 Surface imprinting of proteins: from mechanism to application, YANTIAN WANG, STEFFEN MUELLER, JONATHAN SOKOLOV, Stony Brook University, KALLE LEVON, Polytechnic University, BASIL RICAS, MIRIAM RAFAILOVICH, Stony Brook University — Protein adsorption properties on different surfaces have been of great interest due to their importance in biomedical applications. In this study, adsorption of proteins on gold, thiol self-assembled monolayer (SAM), and molecularly imprinted thiol SAM was studied. Alkaline phosphatase (AP), an enzyme that can catalyze p-nitrophenyl phosphate and produce a yellow end product which has light absorbance at 405nm, was co-adsorbed with 11-mercapto-1-undecanol to fabricate the imprinted surface. Different washing methods were used to remove AP and create re-adsorption sites. The adsorption amount of AP before and after washing was measured by spectrophotometer after enzyme reaction. Re-adsorption of AP onto the three substrates was measured by spectrophotometer after enzyme reaction. Re-adsorption of AP onto the three surfaces was compared and showed that the imprinted surface re-bound the protein molecules at the template site. Potentiometric response of the three substrates to AP was measured at different pH, the charge effect on the potential response was studied. The selective binding of the template proteins made it a useful technique as a protein sensor.
K1.00296 Single Molecule Optical Signal Comparison of Fluorescent Molecules and Raman Active Nanopores. EDWARD ALLGEYER, University of Maine Department of Physics, ADAM PONGAN, GARY CRAIG, MICHAEL MASON, University of Maine Department of Chemical Engineering. MASON LAB GROUP TEAM — In recent years various enhancement techniques have been used to greatly improve the effective cross section of all flavors of raman spectroscopy. Further, coupling specific probe molecules to metal nanoparticles allows for a nanoprobe with an enhanced effective raman cross section making raman probes a viable technique for imaging and spectroscopy in biological and material systems. However, it has been claimed that intensity variations of raman nanopores are to large for raman nanopores to be useful. Here we report on a study of intensity variations of novel raman active nanoprobes and contrast this with intensity variations of typical single molecule fluorescent probes. In both cases an intensity distribution is built from the single molecule level. 

K1.00297 Atomic Force Microscope Investigations of Biofilm-Forming Bacterial Cells Treated with Gas Discharge Plasmas1. KURT VANDERVOORT, ANDREW RENSHAW, NINA ABRAMZON, Physics Department, California State Polytechnic University, Pomona, GRACIELA BRELLES-MARINO, Biological Sciences Department, California State Polytechnic University, Pomona — We present investigations of biofilm-forming bacteria before and after treatment from gas discharge plasmas. Gas discharge plasmas represent a way to inactivate bacteria under conditions where conventional disinfection methods are often ineffective. These conditions involve bacteria in biofilm communities, where cooperative interactions between cells make organisms less susceptible to standard killing methods. Chromobacterium violaceum were imaged before and after plasma treatment using an atomic force microscope (AFM). After 5 min. plasma treatment, 90% of cells were inactivated, that is, transformed to non-culturable cells. Results for cell surface morphology and micromechanical properties for plasma treatments lasting from 5 to 60 minutes were obtained and will be presented. 

1This work was supported by the National Science Foundation under Grant No. 0406533 and by the California State University Program for Education and Research in Biotechnology (CSuperb).

K1.00298 Electrostatic perturbation in neurons and endothelial cells under stress using Atomic Force Microscopy-assisted Electrostatic Nanolithography. VICTORIA NEDASHKIVSKA, SERGEI LYUKSYUTOV, The University of Akron, LOIS-MAY BEZUIDENHOUT, CORNELIS VAN DER SCHYF, NEUOCOM — The morphological and membrane properties of neuronal and vascular endothelial cells need to be studied to reveal their possible role in neurodegeneration after injury. Atomic Force Microscopy Electrostatic Nanolithography (AFMEN) offers an opportunity to measure cellular perturbations during stress conditions. AFMEN is based on electrostatic manipulations of macromolecules and biological tissues at a nanoscale level which generates electric fields of the order of magnitude $10^{-9}$ - $10^{-12}$ V m$^{-1}$ and studies membrane changes in vitro cell culture systems. Two cell culture systems were selected based on their ability to represent neurons on the one hand, and vascular epithelial cells differentiated to model the blood-brain barrier, on the other. The imaging was completed for cells in wet (natural) and also in dry conditions. Changes in membrane behavior will be compared between stressed cells and controls that have not undergone exposure to pathologic conditions. 

K1.00299 Ballistics and Biophysics of Fatal Lesion in Thorax. SAAKI J. SHAIBANI, Independent Modeling, Algorithms & Analytical Studies (IMAAS) — The examination of body-related factors does not always provide the level of insight required to resolve the mechanism of death for major chest injury. Indeed, many autopsy findings are limited when environmental information is either not available at all or is incomplete. Such was the case when a gunshot wound was inflicted upon a standing adult male whose torso was rotated by a forward pitch and a rightward yaw. Highly accurate values for these angles were derived by a process independent from any standard medical approach, along with precise measurements for various anatomical landmarks, so that a meticulous analysis could be performed to determine all plausible bullet trajectories. A combination of physics and medicine then allowed only one viable set of conditions to be identified. The interdisciplinary nature of the research described here was responsible for its success; without such a collaborative study, a full understanding of the relevant issues could not have emerged. Physics-based techniques can also be of benefit in many other applications when the appropriate protocol is defined properly and then implemented correctly.

K1.00300 How are static magnetic fields detected biologically? . LEONARD FINEGOLD, Department of Physics, Drexel University — There is overwhelming evidence that life, from bacteria to birds to bats, detects magnetic fields, using the fields for orientation or navigation. Indeed there are recent reports (based on Google Earth imagery) that cattle and deer align themselves with the earth’s magnetic field. [1]. The development of frog and insect eggs are changed by high magnetic fields, probably through known physical mechanisms. However, the mechanisms for eukaryotic navigation and alignment are not clear. Persuasive published models will be discussed. Evidence, that static magnetic fields might produce therapeutic effects, will be updated [2]. 


K1.00301 Raman Spectroscopy Study of Prostatic Adenocarcinoma Bulk Tissues S. DEVPURA, H. DAI, J.S. THAKUR, R. NAiK, A. CAO, A. PANDYA, G.W. AUNER, Wayne State University, F. SARKAR, W. SAKR, Karmanos Cancer Institute, V. NAiK, University of Michigan-Dearborn — Prostate cancer is one of the most common types of cancer among men. The mortality rate for this disease can be dramatically reduced if it can be diagnosed in its early stages. Raman spectroscopy is one of the optical techniques which can provide fingerprints of a disease in terms of its molecular composition which changes due to the onset of disease. The aim of this project is to investigate the differences in the Raman spectra to identify benign epithelium (BE), prostatic intraepithelial neoplasia (PIN) and adenocarcinoma of various Gleason grades in archived bulk tissues embedded in paraffin wax. For each tissue, two adjacent tissue sections were cut and dewaxed, where one of the sections was stained using haematoxylin and eosin for histological examination and the other unstained adjacent section was used for Raman spectroscopic studies. We have collected Raman spectra from 10 prostatic adenocarcinoma dewaxed tissue sections using Raman microscope (785 nm excitation laser). The data were analyzed using statistical methods of principal component analysis and discriminant function analysis to classify the tissue regions. The results indicate that Raman Spectroscopy can differentiate between BE, PIN and Cancer regions.

K1.00302 Biophysical modeling of mismatch repair proteins1. FREDDIE SALSbury, Wake Forest University — Mismatch repair proteins play a vital role in the biology of cancer due to their dual functions as repair proteins and as sensors of DNA damage. Computational modeling of mismatch repair proteins in conjunction with biological experimentation has demonstrated the role of long-range communication in the functions of these proteins. Furthermore, different conformations have been shown to be associated with different cellular functions, and these differences are being exploited in drug discovery. The latest results in this modeling will be presented. 

1 Acknowledge support from the Translational Sciences Institute at WFU
K1.00303 *In vivo* determination of the structure of oligomers of a G protein-coupled receptor.

SASMITA RATH1, VALERICA RAICU, Department of Physics, University of Wisconsin, Milwaukee, WI 53211 — Resonance Energy Transfer (RET) is a process of nonradiative energy transfer between a donor and an acceptor molecule, which is widely used for studies of protein-protein interactions in living cells. Here we report on the results of a spectrally-resolved two-photon microscopy study of image-pixel level RET in yeast cells (*S. cerevisiae*) expressing a G-protein-coupled receptor called Sterile 2 α factor protein (Ste2P). The number of pixels showing RET were plotted against the RET efficiency to obtain distributions of RET efficiency in the cells. These distributions were simulated with models for plausible geometries and sizes of protein complexes (V. Raicu, 2007, *J. Biol. Phys.* 33:109–127). From all the models tested we found that a parallelogram-shaped tetramer is the most likely structure for the Ste2p oligomers.

1 Corresponding author

Tuesday, March 17, 2009 2:30PM - 5:30PM —

Session L1 DPOLY: John H. Dillon Medal Symposium in Honor of Venkat Ganesan

Spirit of Pittsburgh Ballrom A

2:30PM L1.00001 Dillion Medal Prize Lecture. VENKAT GANESAN, The University of Texas at Austin — Many aspects of polymer research have undergone a paradigm shift in the past decade, with an increased emphasis on technological applications which propose the use of materials and devices created by controlling matter from the atomic scales to the bulk commodity level. This talk will focus on multicomponent polymeric materials (block copolymers, rod-coil polymers and mixtures like polymer blends and polymer nanocomposites), which have played a central role in enabling this paradigm shift in the context of polymeric materials. In this talk, I will discuss our recent researches on developing simulation tools that can predict the structure, morphology and flow behavior of such multicomponent polymers. In contrast to conventional ("particle-based") Monte Carlo and Molecular dynamics approaches, our methods work at a coarse-grained level of the system to predict the thermodynamics and dynamics of such multicomponent materials. This talk will focus on an outline of the simulation strategies and present some results concerning both the equilibrium and dynamical properties of such materials.

3:06PM L1.00002 Chain Stretching and Order-Disorder Transitions in Block Copolymer Monolayers and Multilayers. EDWARD J. KRAMER, VINDHYA MISHRA, GILA E. STEIN, KAREN E. SOHN, SUMI HUR, GLENN H. FREDRICKSON, UCSB, ERIC W. COCHRAN, Iowa State University — Both monolayers of block copolymer cylinders and spheres undergo order to disorder transitions (ODT) at temperatures well below those of the bulk. Monolayers of PS-b-P2VP cylinders undergo a “nematic” to “isotropic” transition at temperatures about 20 K below the bulk ODT while monolayers of PS-b-P2VP with P2VP spheres undergo a 2D crystal to hexatic transition at temperatures about 10 K below the bulk ODT. Bilayers of each structure disorder at temperatures well above that of the monolayers. While one is tempted to attribute all of the difference to the fact that ordered monolayers are quasi 2 dimensional while bilayers are not, an alternative explanation exists. In the cylinder monolayer the corona PS chains must stretch to fill a nearly square cross-section domain rather than a hexagonal one in the bulk, while the corona PS chains in a sphere monolayer must stretch to fill a hexagonal prism rather than an octahedron in the bulk. The more non-uniform stretching of the chains in the monolayer should increase its free energy and decrease its order-disorder temperature.

3:18PM L1.00003 Free Energy Estimation in Field-Theoretic Simulations. GLENN FREDRICKSON, ERIN LENNON, KIRILL KATSOY, UC Santa Barbara — A new technique is presented for computing absolute and relative free energies of polymeric fluids in the context of field-theoretic simulations. Complex Langevin sampling is combined with a thermodynamic integration scheme to provide access to free energies of homogeneous and inhomogeneous polymer phases. The scheme utilizes a harmonic crystal reference state whose free energy can be computed analytically. The method is demonstrated in the context of the order-disorder transition of diblock copolymer melts.

3:30PM L1.00004 Directed Crystallization in polymer solutions. MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Theoretical considerations of amyloid fibrillation in protein solutions and polymer-mediated crystallization of nanoparticles will be presented.

3:42PM L1.00005 The O52 Network by Molecular Design: CEC D Tetra block Terpolymers. FRANK S. BATES, MICHAEL BLUEMLE, GUILLAUME FLEURY, TIMOTHY LODGE, U. Minnesota — Varying the length of poly(dimethylsiloxane) in poly(cyclohexylethylenethylene-b-ethylene-b-cyclohexylethylenylene-b-dimethylsiloxane) (CECD) terablock terpolymers between 0 and 20% produces the sequence of ordered phases: cylindrical-to-network-to-cylindrical. Small-angle X-ray scattering and transmission electron microscopy demonstrate Pnma space group symmetry and a unique network morphology stabilized by the asymmetric molecular architecture and block interactions. These results establish a new design principle for the generation of triply periodic and multiply continuous nanostructured soft material.

3:54PM L1.00006 Suppression of Segmental Relaxation as the Origin of Strain Hardening in Polymer Glasses. KENNETH SCHWEIZER, KANG CHEN, University of Illinois — A nanometer scale dynamical theory is proposed for the post-yield large amplitude strain hardening phenomenon in polymer glasses. The physical picture is that external deformation induces anisotropic chain conformations which modifies interchain packing, resulting in density fluctuation suppression and intensification of localizing dynamical constraints and activation barriers. The strain amplitude dependence of the resulting stresses are well described by classic rubber elasticity form. However, the hardening stress is of interchain origin and arises primarily from prolongation of segmental relaxation, not single strand entropic elasticity. Theoretical predictions for the magnitude, temperature and deformation rate dependence of the hardening modulus are consistent with experiments and simulations.

4:06PM L1.00007 Disappearance of high frequency modes in polymer dilute solution viscoelasticity. RONALD LARSON, University of Michigan, SEMANT JAIN, Praxair — We address the problem of the “missing modes” in the high frequency rheology of dilute polymer solutions. According to the Rouse-Zimm theory, the slow viscoelastic response of dilute polymers is dominated by the collective motion of the chain, as described by a bead-spring model. However, one expects this description to break down at high frequencies at which chain motion on scales too small to be represented by beads and springs should be evident; this motion should be controlled by rotations of individual backbone bonds of the polymer. The viscoelastic response produced by these “local modes” is observable in polymer melts; however, for dilute polymer solutions, the “local modes” are absent from viscoelastic spectra, as shown by Schrag and coworkers (Peterson, et al., *J. Polym. Sci.* B, 39:2860 (2001)). Here we address this problem by directly simulating single polymer chains using Brownian dynamics simulations, with realistic bending and torsional potentials. We show using these simulations that the “missing modes” result from barriers to bond rotation that make the chain “dynamically rigid” at high frequencies. As a result, the “dynamical Kuhn length” of the chain exceeds the static one, and the chain at high frequencies is not able to explore local conformations as fast as would be needed for their relaxation to contribute to the mechanical relaxation spectrum.
4:18PM L1.00008 Polymer Conductivity through Particle Connectivity. YUEH-LIN LOO, Princeton University — To promote solution processability of conductive polymers, polymer acids, instead of small-molecule acids, are frequently used as dopants. Generally, the conductive polymer is synthesized in the presence of the polymer acid; sub-micron size particles that are electrostatically stabilized result during polymerization. We discovered that the molecular characteristics of the polymer acid have great implications on the structure of these conductive polymer particles. Templating the synthesis of the conductive polymer with a higher molecular weight polymer acid results in larger particles, and templating with a polymer acid having a larger molecular weight distribution results in a large size distribution in the particles. Because conduction in such conductive polymers is governed by how these particles pack, we show that the macroscopic conductivity of these films is dictated by a single parameter, i.e., the particle density, that is reducible from the various molecular characteristics of the polymer acid we explored. In the specific case of polyaniline that is doped with poly(2-acylamido-2-methyl-1-propane sulfonic acid), the particles are structurally and chemically inhomogeneous. The conductive portions of the polymer preferentially segregate to the particle surface. Conduction in these materials are therefore mediated by the particle surface and conductivity thus scales superlinearly with particle surface area per unit film volume.

4:30PM L1.00009 Modeling the Self-Assembly of Nanoparticle Amphiphiles. SANAT KUMAR, Columbia University, ATHANASSIOS PANAGIOTOPoulos, Princeton University — We demonstrate that spherical nanoparticles, uniformly grafted with macromolecules, robustly self-assemble into a range of anisotropic superstructures when they are dispersed in the corresponding homopolymer matrix. Theory and simulations both suggest that this self-assembly process reflects a balance between the energy gain when particle cores approach and the entropy of distorting the graft polymers. The effectively directional nature of the particle interactions is thus a many-body emergent property.

4:42PM L1.00010 Confinement Effects on Polymer Dynamics in Nanocomposites. RAMANAN KRISHNAMOORTI, University of Houston, TIRTHA CHATTERJEE, UC Santa Barbara, Mansour Abdolbaki, University of Houston, Madhusudan Tyagi, NIST — The dynamics of polymers in systems with dispersed nanoparticles is studied using inelastic and quasi-elastic neutron scattering. In this study, the role of confinement between nanoparticles and the role of nanoparticle topology are examined by considering dispersions with spherical C60 buckyballs, rod-like single walled carbon nanotubes and plate-like graphene. The polymers examined here include bisphenol A epichlorohydrin and bisphenol F epichlorohydrin. Significant changes in the dynamics of the polymer are observed and these will be examined in the context of mode coupling theories.

4:54PM L1.00011 Long-time dynamics of chains in polymer nanocomposites. Peter Green, University of Michigan — In polymer nanocomposites (PCNs), the presence of the nanoparticles has a marked effect on the dynamics and the Tg. In one limit, the chains become strongly attached to the particles, and two glass transitions, and bimodal dynamics, may be observed. In the other, where the chain/particle interactions are weak, the chain friction factor, z(T), can undergo significant changes, manifested in the translational diffusion and viscosity. In the polystyrene-methacrylate (PMMA)/C60 system, the dynamics slow down, accompanied by an increase in the glass transition. At the same time, the temperature dependence of the relaxations remains the same as pure PMMA. In polystyrene/Au-thiol capped PS ligands, the dynamics and the glass transition could be induced to increase or decrease, through manipulation of molecular parameters in the system. In this presentation, we propose a mechanism to describe translational diffusion and Tg in PCN systems in which the polymer chain/nanoparticle interactions are weak.

5:06PM L1.00012 Self-Assembly of Conjugated Rod-Coil Block Copolymers for Photovoltaic Applications. R. A. Segalman, B.D. Olsen, Y. Tao, B. McCulloch, UC Berkeley and Lawrence Berkeley National Laboratories — The phase behavior of conjugated rod-coil block copolymers is significantly different from that of traditional block copolymers due to the interplay between liquid crystalline interactions of the rod blocks and microphase separation of the rods and coils. A universal phase diagram for rod-coil diblock copolymers depends on the strengths of the rod aligning interactions and the rod-coil repulsive interactions as well as the geometrical ratio of rod volume to coil and aspect ratios. In this talk, the experimental phase diagram of a weakly segregated model block copolymer will be compared to that predicted by self-consistent field theory. Conjugated rod-coil block copolymers with electron donating and accepting blocks are promising for photovoltaic applications. The self-assembly of poly(thiophene-b-acylate perylene diimide) block copolymers as well as block copolymer-nanocrystal composites result in photovoltaic active layers with controllable degrees of order. We demonstrate that short range order on the nanoscale is beneficial to device performance.

5:18PM L1.00013 Confinement Effects on Glassy-State Polymer Behavior in Thin Films, Nanocomposites, Tethered Nanoparticles, and Nanostructured Systems. John Torkelson, Perla Ritigstein, So Young Kim, Rodney Priestley, Connie Roth, Manish Mundra, Northwestern University — Confinement of polymers at the nanoscale and even the microscale can lead to significant deviations in glass transition temperature, physical aging rate, and alpha-relaxation dynamics from bulk polymer behavior. Here we illustrate how model experiments involving several techniques applied to simple, thin polymer films help us to understand and predict qualitatively or semi-quantitatively the glassy-state response of more complex, confined systems, including nanocomposites, tethered nanospheres, nanostructured homopolymer films, and nanostructured systems consisting of more than one polymer component. We shall illustrate how the glass transition temperature can be altered by as much as 60 K and how physical aging can be nearly totally suppressed via confinement. The discovery of new confinement effects and implications for new applications of confined polymer systems will be discussed.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L2 DCMP: Buckley and Lilienfeld Prize Spirit of Pittsburgh Ballroom BC

2:30PM L2.00001 Oliver E. Buckley Prize Talk: Birth of tunnel magnetoresistance and its development. Terunobu Miyazaki, 2-1 Katahira, Aoba-ku, Sendai 980-8577 — Nowadays usually we use the word, tunnel magnetoresistance, but it required a long time to combine both words tunnel and magnetoresistance. The study of tunnel junction may originate p-n junction studied first around 1950. On the other hand, magnetoresistance effect was reported first in 1857 which was about 100 years earlier than the start of tunnel junction study. The research of tunnel magnetoresistance has been mainly developed first for Al-oxide tunnel barrier junctions and made a big progress by the appearance of MgO barrier junctions for both basic research and applications. More recently Heusler electrode tunnel junctions exhibits a large TMR ratio up to about 750 %, so we will focus on the Heusler electrode junctions and also application of tunnel magnetoresistance junctions.

3:06PM L2.00002 Oliver E. Buckley Prize Talk: Spin-dependent tunneling. Robert Meservey, MIT

Francis Bitter Magnet Laboratory — This abstract not available.
3:42PM L2.00003 Oliver E. Buckley Prize Talk: Spin polarized tunneling and tunnel magnetoresistance – Learning from the past and moving forward\(^1\), JAGADEESH MOODERA, Massachusetts Institute of Technology — Electron tunneling phenomenon has contributed enormously to our understanding of various branches of physics over the years. The technique of spin polarized tunneling (SPT), sensing the spin polarization of tunneling electrons using a superconducting spin detector, discovered by Meservey and Tedrow in the early seventies has been successfully utilized over the years to understand many aspects of magnetism and superconductivity. Electrical spin injection/detection in a semiconductor is strongly believed to succeed through such an approach. The successful observation of a large change in tunnel current in magnetic tunnel junctions (MTJ) in the mid nineties has brought extreme activity in this field – both from fundamental study as well as extensive application in mind (as sensors, nonvolatile memory devices, logic elements etc.). From the early history of this field that led to the discovery of room temperature TMR effect to the observation of many novel phenomena to the exciting recent work on spin filtering, spin transport in semiconductors to toggling of the superconducting state with spin current will be highlighted and reviewed. Work done in collaboration with Drs. Meservey and Tedrow, PhD students, postdoctorals, as well as high school students and undergraduates. NSF, ONR, DARPA and KIST-MIT project funds supported the research over the years.

\(^1\) NSF, ONR, DARPA and KIST-MIT project funds supported the research over the years.

3:42PM L2.00004 Oliver E. Buckley Prize Talk: Discovery and exploration of spin-dependent tunneling\(^1\), PAUL TEDROW\(^2\), Francis Bitter Magnet Laboratory, MIT — Experiments on thin-film superconductors in intense magnetic fields by R. Meservey and P. M. Tedrow led to the discovery of spin-polarized tunneling. Measurements of the critical magnetic of very thin aluminum films for temperatures down to 0.45 K verified that spin-orbit scattering had to be included in the BCS description of the critical field. Theory predicted a first order transition at low temperature, and, although measurements of the shape of the resistive transition of the films strongly implied the existence of such a transition, magnetic field-dependent tunneling measurements of the energy gap of the aluminum were undertaken to observe directly the first-order nature of the transition. Splitting of the superconducting density of states by the applied magnetic field, i.e., spin-dependent tunneling, was observed in these measurements. Subsequent tunneling experiments demonstrated the spin polarization of tunnel currents from ferromagnets. The extension of these tunneling studies to include a wide range of superconductors and magnetic materials produced new qualitative and quantitative information about the behavior of conduction electron spins in such materials. Although experimental technique and theory have improved from these early times, there remain unanswered questions concerning electron tunneling into ferromagnets. An overview of these early experiments will be presented\(^3\).

\(^1\) We acknowledge the theoretical support by Dr. Brian Schwartz, Professors Peter Fulde and Dierk Rainer, the work of Dr. Jagadeesh Moodera, the contributions of graduate students and technical staff, and the financial support of the AFOSR, NSF, and NASA.

\(^2\) Buckley Prize

\(^3\) A review can be found in R. Meservey and P. M. Tedrow, Physics Reports 238, 175 (1994).

4:54PM L2.00005 Julius Edgar Lilienfeld Prize: The RG and me: love at first bite\(^1\), RAMAMURTI SHANKAR, Yale — From the time I took the first bite out of that cut-off, I have been in love with the Renormalization Group, returning to it over and over again to apply it to classical and quantum problems, in clean as well as disordered systems. This talk, aimed at non-experts, introduces and illustrates the RG ideas, with a favorite application, understanding Landau’s fermi liquid.

\(^1\) Supported by NSF grant DMR- 0103639

Tuesday, March 17, 2009 2:30PM - 4:54PM — Session L3 DCMP: Fe-based Superconductors: Competing Orders 301/302

3:06PM L3.00001 Competing orders and spin density wave instabilities in FeAs-based systems , NANN LIN WANG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190 — The discovery of superconductivity with T\(_c\) up to 55 K in layered FeAs-based compounds has generated tremendous interest in the scientific community. Except for relatively high T\(_c\), the Fe pnictides display many interesting properties. Among others, the presence of competing orders is one of the most intriguing phenomena. In the early stage of our study on the compounds, we identified a spin-density-wave (SDW) ordered state for the parent compound with a stripe (or collinear) type spin structure based on the transport, specific heat, optical spectroscopy measurements and the first- principle calculations. The proposed spin structure is in a nesting of the Fermi surfaces is confirmed by subsequent neutron experiments. However, it could also be explained by a local superexchange picture. In this talk I shall focus on our recent optical data on single crystal samples, trying to address the debating issue about itinerant or localized approaches to the SDW order. We found that the undoped compounds are quite metallic with relatively high plasma frequencies above T\(_{SDW}\). Upon entering the SDW ordered state, a large part of the Drude component is removed by the gapping of Fermi surfaces. Meanwhile, the carrier scattering rate is even more dramatically reduced. Those observations favor an itinerant description for the driving mechanism of SDW instability. Nevertheless, our experiments also indicate that Fe pnictides are not simple metals. A high energy gap-like feature is present even above T\(_{SDW}\), which seems to be linked with the antiferromagnetic spin fluctuations. For the superconducting samples, a superconducting pairing energy gap is clearly observed in the far-infrared reflectance measurement. The Ferrell-Glover- Tinkham sum rule is satisfied at a low energy scale. Work done in collaboration with: G. F. Chen, J. L. Luo, Z. Fang, X. Dai, W. Z. Hu, J. Dong, G. Li, Z. Li, P. Dai, J. Lynn, H. Q. Huang, J. Singleton.

3:30PM L3.00002 Magnetic order close to superconductivity in the iron-based layered RFeAsO\(_x\)F\(_{1-x}\) (R = La, Ce) systems , PENGCHENG DAI, Univ of Tennessee, Knoxville — No abstract available.

3:42PM L3.00003 Competing Magnetic Interactions, Structural Phase Transition, and the Unprecedented Giant Coupling of Fe-spin State and the As-As Interactions in Iron-Pnictide , TANER YILDIRIM, NIST and University of Pennsylvania — From all-electron fixed-spin-moment calculations \([1]\), we showed that the ferromagnetic and checkerboard antiferromagnetic ordering in LaOFeAs were not stable and the stripe Fe-spin configuration (i.e. SDW) was the only stable ground state. The main exchange interaction between Fe ions are large, antiferromagnetic, and frustrated. The magnetic stripe SDW phase breaks the tetragonal symmetry, removes the frustration, and causes a structural distortion. We unravel surprisingly strong interactions between arsenic ions, the strength of which is controlled by the Fe-spin state in an unprecedented way \([2]\). Reducing the Fe-magnetic moment, weakens the Fe-As bonding, and in turn, increases As-As interactions, causing giant reduction in the c-axis. For Ca\(_2\)Fe\(_2\)As\(_2\) system, this reduction of c-axis with the loss of the Fe-moment is as large as 1.4 Å, an unheard of giant coupling of local spin-state of an ion to its lattice. Since the calculated large c-reduction has been recently observed only under high-pressure, our results suggest that the iron magnetic moment should be present in Fe-pnictides at all times at ambient pressure. Implications of these findings on the mechanism of superconductivity in iron-pnictides will be discussed.


Extending the NMR work to lower temperatures we find evidence for a deviation of the T³⁻¹ behaviour of the spin lattice relaxation, which would agree with the extended s-wave symmetry suggested in recent theoretical work. In the paramagnetic normal state, NMR on all three nuclei shows that the local electronic susceptibility rises with increasing temperature. This had led to suggest the presence of a pseudogap, which I will discuss in detail. The scaling of all NMR shifts with respect to the macroscopic susceptibility indicates that there is no apparent multiband effect through preferential hyperfine couplings. Relaxation measurements indicate a similar temperature-dependence for (T₁T)⁻¹ and suggest that the dynamical susceptibility changes uniformly in q space with varying temperature. The transport properties show some striking similarities to the findings in cuprates [6] and, finally, susceptibility [4] as well as NMR studies point to the antiferromagnetic fluctuations, whose relevance is also discussed in many theoretical models of the superconducting pairing mechanism. In collaboration with Hans-Joachim Grafe, Christian Hess, Rüdiger Klingeler, Günther Behr, Agnieszka Kondrat, Norman Leps, and Guillaume Lang, IFW Dresden; Hans-Henning Klauss, TU Dresden; and Hubertus Luetkens, PSI Villigen.

References:

Tuesday, March 17, 2009 2:30PM - 5:30PM –
Session L4 COM: The Dynamics of Diversity in Astrophysics 306/307

2:30PM L4.00001 Probing Beyond Einstein: The Joint Dark Energy Mission, LARRY GLADNEY, Department of Physics and Astronomy, University of Pennsylvania — The discovery of the acceleration of the expansion of the universe in 1998 represents perhaps the most profound challenge to our current understanding of physics and astronomy. The observation of acceleration requires either that more than 70% of the contents of the universe be an exotic form of energy (the so-called “dark energy”) or that there is a flaw in general relativity. The failure of present theories to convincingly explain the effect leads many experts to expect that elucidating the cause of the expansion will lead to fundamental breakthroughs that impact cosmology, astrophysics, and particle physics. The NASA/DOE Joint Dark Energy Mission (JDEM) will be the first of the Beyond Einstein probes. This mission will determine whether the acceleration of the expansion of the universe has varied over time in an attempt to determine the equation of state for dark energy or whether predictions from general relativity fail to adequately explain the acceleration. This talk will present the rationale for a space-based study of dark energy and the techniques likely to be used as part of JDEM.

3:06PM L4.00002 Thermodynamics of the Universe, SAMINA MASOOD, University of Houston-Clear Lake — Properties of fundamental particles are changed in hot and dense media. This fact helps to determine the thermodynamics of the universe from the changed properties of particles in the early universe. We study the behavior of light particles including neutrinos in thermal media to find out the details about the early universe. The neutrino oscillation and the magnetic moment of neutrino, however, do not seem to change significantly enough in thermal background to fully justify the big bang model. We have to look for other properties of neutrinos including entanglement to support the standard model.

3:42PM L4.00003 Space Weather and Global Warming, GEORGE CARRUTHERS, Naval Research Laboratory — This presentation will give discussions of the broad topic of Space Weather, and of Global Warming (these have some associations, as well as differences). Both have the Sun as the major energy source; short-term differences in solar activity are the sources of space weather (which affects the entire solar system, not just our Earth), whereas global warming is a longer-term event which depends on both the Sun and on the lower regions of the Earth’s atmosphere, and (more recently) human activities. In particular, the major gas of interest for global warming is the addition of carbon dioxide to the atmosphere by combustion of coal and oil. Means for decreasing the latter will be discussed, as well as of the effects of space weather on further human exploration of near-Earth and solar system environments.

4:18PM L4.00004 The Accelerating Universe, RUTH DALY, Penn State University — Several different types of observations indicate that the universe is accelerating at present, and was decelerating in the recent past. These observations and a model-independent analysis of the data will be discussed. The model-independent, or assumption-free, data analysis method will be applied to determine the expansion and acceleration rates of the universe as functions of redshift, independent of the contents of the universe and of a theory of gravity. A new model-independent function, the dark energy indicator, which provides a measure of deviations of the equation of state at different redshift from predictions in the standard model, will be presented and discussed. The data will be used to solve for the pressure, energy density, equation of state, and potential and kinetic energy densities of the dark energy as functions of redshift without assuming a model or functional form for the dark energy.

4:54PM L4.00005 Participation and Research of Astronomers and Astrophysicists of Black African Descent, HAKEEM OLUSEYI, Florida Institute of Technology — No abstract available.

Tuesday, March 17, 2009 2:30PM - 5:30PM
Session L5 DCMP: Competing Ground-States and Novel Excitations in Strongly Correlated Metals 401/402
2:30PM L5.00001 Quantum criticality in a cubic heavy fermion cage compound

Silke Paschen, Vienna University of Technology — Matter at the absolute zero in temperature may reach a highly exotic state: Where two distinctly different ground states are separated by a second order phase transition the system is far from being frozen; it is undecided in which state to be and therefore undergoes strong collective quantum fluctuations. Quantum criticality describes these fluctuations, their extension to finite temperatures, and the resulting unconventional physical properties. Heavy fermion compounds have been much investigated in the past few years as model systems. An important recent finding is that in the tetragonal compound YbRh$_2$Si$_2$ [1] a new energy scale vanishes at the quantum critical point and is in addition to the second-order phase transition scale that governs the behavior of conventional quantum critical points [2,3]. New theoretical scenarios can account for this finding if 2-dimensional spin fluctuations are assumed [4]. Here similar behaviour of the new heavy fermion compound Ce$_3$Pd$_{20}$Si$_6$ [5] is discussed in which the cubic crystal structure and the highly symmetric local environment of the Ce atoms in molecular “cages” makes 2-dimensional spin fluctuations rather unlikely.


Financial support of the Austrian Science Fund (project P19458-N16) is gratefully acknowledged.

3:06PM L5.00002 A New Route to Quantum Criticality in Yb$_3$Pt$_4$

Meigan Aronson, Brookhaven National Laboratory/Stony Brook University — The vanishing of magnetic order at a quantum critical point (QCP) is a central feature of virtually all classes of correlated electron systems, and may be accompanied by unconventional ordered states such as superconductivity, and by anomalous critical scattering. Some of the most detailed studies have focused on f-electron heavy electron compounds, and here the picture has emerged that magnetic order requires the formation of moments, provided by the divergence of the quasiparticle mass at the QCP. We combine specific heat, magnetization, and electrical resistivity measurements on the new compound Yb$_3$Pt$_4$, to argue that alternative routes to quantum criticality are also possible. The weakly first order antiferromagnetic transition in Yb$_3$Pt$_4$ can be tuned by field to a critical end point, which is extended to a quantum critical point at 1.62 T. Both the ordered and paramagnetic phases are Fermi liquids at low temperatures, but the quasiparticle mass does not diverge at the QCP. Instead, a divergence of the zero temperature susceptibility and the quasiparticle scattering is observed, controlled by a zero field fixed point and not the nearby QCP. We argue that Yb$_3$Pt$_4$ is the first example of a heavy electron system where magnetic order occurs at the QCP due to increasingly strong quasiparticle interactions, much as is found in $^3$He, Stoner ferromagnets, and spin density wave systems.


Work at Stony Brook University carried out under NSF-DMR-0405961

3:42PM L5.00003 Magnetism and the Fermi surface in heavy fermion metals

Seiji Yamamoto, Rice University — With a plethora of different phases and quantum critical points, heavy fermion materials should reign supreme as the prototype for competing order, a major contemporary theme in condensed matter physics. One key feature that differentiates the types of magnetic phases/critical points is the presence or absence of Kondo screening. This singlet formation is dramatically manifested in the Fermi surface, which provides important experimental insight into the problem. The size of the Fermi surface therefore becomes an important issue. To provide a theoretical basis for the different types of magnetism, we have recently carried out asymptotically exact studies of the Kondo lattice model inside both the antiferromagnetic [1] and ferromagnetic [2] phases. A fundamental aspect of the approach is to map the magnetic Hamiltonian for the local f-moments onto a quantum nonlinear sigma model (QNLSm). The Kondo interaction results in an effective coupling between the QNLsM fields and the conduction electrons. Renormalization group analyses show that the Fermi surface in the corresponding ordered states is small (not incorporating the f-moments) for both the ferromagnetic and antiferromagnetic cases. These results are of relevance to a number of materials, including YbRh$_2$Si$_2$ and CeRu$_2$Ge$_2$, where experimental measurements of magnetotransport and de Haas van Alphen effects [3,4] have provided evidence for the small Fermi surface phases. The implications of our results for the heavy fermion quantum critical points will also be discussed.


4:18PM L5.00004 How Do Heavy Fermions Get Polarized And Die?

Stephen Julian, University of Toronto — In paramagnetic heavy fermion systems the f-spins dissolve into Kondo singlets and reappear within the Fermi volume, producing a “large” Fermi surface populated by heavy quasiparticles. According to theory, when a very large magnetic field is applied to such a system the Kondo singlets are broken and the fully polarized bare f-spins vanish from the Fermi volume, leaving behind a “small” Fermi surface populated by light quasiparticles. How the system passes from the low-field to the high-field limit is not clear. This talk will discuss recent transport and de Haas van Alphen studies of the archetypal heavy fermion compounds CeRu$_2$Si$_2$ [1] and YbRh$_2$Si$_2$ [2], which are interpreted as showing that the f-electron disappears from the Fermi volume via two successive Lifshitz transitions: in the first transition a major spin band sinks below the Fermi level, while in the second a new minority spin band appears at the Fermi level. While this interpretation is in accord with recent theoretical work of Kusminskiy et al. [3], it could be criticized on the grounds that only the first of the two postulated Lifshitz transitions have so far been observed.

References:

4:54PM L5.0005 Electron spin resonance in Kondo systems

Peter Woelfle, Brookhaven National Laboratory — In heavy fermion compounds, in which ferromagnetic correlations appear to be present [1], the spin lattice relaxation and quasiparticle interaction processes.

proteins or other cellular machinery. We also show that it is unlikely to be the result of a hypothetical “open” conformation of the repressor.

short DNA loops (around 95 bp) the experiments show more looping than is predicted by the linear-elasticity model, echoing other recent experimental results.

tethered particle motion (TPM) experiments; e.g. it accounts for all the entropic forces present in such experiments. Our model has no free parameters; it characterizes DNA elasticity using information obtained in other kinds of experiments. It can compute both the “looping J factor” (or equivalently, looping free energy) for various DNA construct geometries and repressor concentrations, as well as the detailed probability density function of bead excursions. We also show a new method to correct observed data for finite camera shutter time. The model successfully reproduces the detailed distributions of bead excursion, including those obtained in TPM experiments, confirming that the repressor tetramer is a rigid body. A new approach for investigating turbulent nonlinear dynamics is presented. The scaling exponents that are observed in the Lagrangian description of turbulence is also presented. The magnetic Reynolds number in the outer core is about 20 times the critical value for sustained dynamo action and the Reynolds number is about $10^7$, implying turbulent conditions. Fluctuations in the turbulence induce continuous changes in the geomagnetic field, including occasional polarity reversals. Geomagnetic polarity reversals have occurred about once every 250 kyr on average over the past 5 Myr, the last reversal occurred around 780 ka and there have been several long constant- polarity superchrons. The axial dipole collapses before a reversal, exposing the complex non-dipolar transition field, then the axial dipole is regenerated in the opposite polarity, the entire process lasting 10-20 kyr. Spontaneous polarity reversals have been observed in at least one liquid sodium dynamo experiment. Downward-extrapolated measurements from Earth-orbiting satellites reveal the axial dipole comes mostly from a few high-latitude concentrated flux spots on the core boundary. About 15% of the core boundary has reversed-direction magnetic field, mostly in the southern hemisphere. Proliferation and growth of reversed flux regions are major reasons why the axial dipole is in decline, decreasing at 10 times its free decay rate and suggesting (to some) that the geomagnetic field may be in early stage of a polarity reversal. 

3:06PM L6.00002 Flows and jets around compact astrophysical objects , JOHN HAWLEY, University of Virginia — No abstract available.

3:42PM L6.00003 Fluid Mechanics of the Geodynamo , PETER OLSON, Johns Hopkins — Fluid dynamical processes in the molten, iron-rich, electrically conducting core sustain Earth’s magnetic field. Convection driven by secular cooling and chemical differentiation is the primary energy source for the geodynamo. Earth’s rotation imparts helicity to the convection, which amplifies the geomagnetic field, balancing losses from Ohmic dissipation. Both the Ekman and Rossby numbers are very small in the outer core, so the convection is partly aligned with the planetary spin axis, which tends to orient the geomagnetic dipole axis in the north-south direction. The magnetic Reynolds number in the outer core is about 20 times the critical value for sustained dynamo action and the Reynolds number is about $10^7$, implying turbulent conditions. Fluctuations in the turbulence induce continuous changes in the geomagnetic field, including occasional polarity reversals. Geomagnetic polarity reversals have occurred about once every 250 kyr on average over the past 5 Myr, the last reversal occurred around 780 ka and there have been several long constant- polarity superchrons. The axial dipole collapses before a reversal, exposing the complex non-dipolar transition field, then the axial dipole is regenerated in the opposite polarity, the entire process lasting 10-20 kyr. Spontaneous polarity reversals have been observed in at least one liquid sodium dynamo experiment. Downward-extrapolated measurements from Earth-orbiting satellites reveal the axial dipole comes mostly from a few high-latitude concentrated flux spots on the core boundary. About 15% of the core boundary has reversed-direction magnetic field, mostly in the southern hemisphere. Proliferation and growth of reversed flux regions are major reasons why the axial dipole is in decline, decreasing at 10 times its free decay rate and suggesting (to some) that the geomagnetic field may be in early stage of a polarity reversal. 

4:18PM L6.00004 Statistics and scaling in magnetohydrodynamic turbulence , WOLF-CHRISTIAN MÜLLER, Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany — The nonlinear cascade of energy is one of the most prominent processes in turbulent systems. The associated self-similarity of two- point statistics leads to the appearance of inertial-range scaling laws, e.g. in the energy spectrum of turbulence. The scaling exponents that are observed in experiments or direct numerical simulations allow to verify the validity of cascade phenomenologies. Currently, controversial findings have led to a confusing situation in the phenomenological understanding of nonlinear inertial-range dynamics of magnetohydrodynamic turbulence which is discussed using recent results of direct numerical simulations. A new approach for investigating turbulent nonlinear dynamics which is based on the Lagrangian description of turbulence is also presented. 

4:54PM L6.00005 Turbulence in the interstellar and interplanetary medium , GARY ZANK, University of Alabama — No abstract available.
3:06PM L7.00002 Modulation of membrane mechanical properties by Sar1, a vesicle trafficking protein. , RAGHVUEER PARTHASARATHY, University of Oregon — The trafficking of cargo in cells involves dramatic changes in membrane shape and topology. Though trafficking is widely studied and the identities and interactions of the responsible proteins are well mapped, remarkably little is known about the mechanics involved. We focus on Sar1, the key regulator of the coat protein complex II (COPII) family that ferries newly synthesized proteins from the ER to the Golgi. Sar1 is the only member of the COPII coat that interacts directly with the ER lipid bilayer membrane. It has an amphiphatic N-terminal helix; when Sar1 is GTP-bound, the helix is exposed and the hydrophobic semi-cylinder can insert into the bilayer. To investigate whether Sar1 has a role beyond merely localizing the other COPII proteins, we directly measure the force involved in membrane deformation as a function of its presence or absence, using optically trapped microparticles to pull tethers from lipid membranes whose composition and large surface area mimic the composition and geometry of the ER. Tether measurements allow extraction of the membrane bending modulus, the parameter that governs the energetics of deformation. We find that the bending modulus measured in the presence of Sar1 with a non-hydrolyzable GTP analogue is half that measured without Sar1 or with Sar1-GDP. These results reveal a paradigm-altering insight into COPII trafficking: Sar1 actively alters the material properties of the membranes it binds to, lowering the energetic cost of curvature generation.

3:42PM L7.00003 ABSTRACT WITHDRAWN —

4:18PM L7.00004 “Double Bubble” and other trouble with DNA looping, ALEXEI TKACHENKO, Physics Department, University of Michigan — DNA looping is essential for such biological processes as regulation of gene expression and DNA packaging into nucleosomes. Classical theory of looping, based on the elastic description of DNA, was proposed more than two decades ago by Shimada and Yamakawa. However, a number of puzzles related to the problem remain largely unresolved to date. For instance, DNA loops in nature tend to be significantly shorter than the optimal one once predicted theoretically, and the looping probability appears to be much larger. Even in vitro experiments conflict with each other and with the theory. In my talk, I will review a number of mechanisms which may be responsible for these discrepancies, and which add complexity to the overall problem. I will briefly discuss possible roles of bending-induced and protein-induced structural defects (such as kinks and bubbles), as well as effects of boundary constraints. I will then focus on two phenomena: the effect of sequence disorder, and the loop formation in a supercoiled DNA. The former results in the lack of self-averaging of looping probabilities. The supercoiling may explain the smaller optimal loop size observed in vivo.

4:54PM L7.00005 Push or Pull? – Cryo-Electron Microscopy of Microtubule’s Dynamic Instability and Its Roles in the Kinetochores, HONG-WEI WANG, Department of Molecular Biophysics and Biochemistry, Yale University — Microtubule is a biopolymer made up of alpha-beta-tubulin heterodimers. The tubulin dimers assemble head-to-tail as protofilaments and about 13 protofilaments interact laterally to form a hollow cylindrical structure which is the microtubule. As the major cytoskeleton in all eukaryotic cells, microtubules have the intrinsic property to switch stochastically between growth and shrinkage phases, a phenomenon termed as their dynamic instability. Microtubule’s dynamic instability is closely related to the types of nucleotide (GTP or GDP) that binds to the beta-tubulin. We have biochemically trapped two types of assembly states of tubulin with GTP or GDP bound representing the polymerizing and depolymerizing ends of microtubules respectively. Using cryo-electron microscopy, we have elucidated the structures of these intermediate assemblies, showing that tubulin protofilaments demonstrate various curvatures and form different types of lateral interactions depending on the nucleotide states of tubulin and the temperature. Our work indicates that during the microtubule’s dynamic cycle, tubulin undergoes various assembly states. These states, different from the straight microtubule, lend the highly dynamic and complicated behavior of microtubules. Our study of microtubule’s interaction with certain kinetochore complexes suggests that the intermediate assemblies are responsible for specific mechanical forces that are required during the mitosis or meiosis. Our discoveries strongly suggest that a microtubule is a molecular machine rather than a simple cellular scaffold.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L8 DCMP GSNP: Jamming at Nonzero Temperature and Stress 414/415

2:30PM L8.00001 Simple scaling of the glass transition temperature with pressure 1, NING XU, University of Pennsylvania and University of Chicago — Zero-temperature packings of frictionless spheres have been used as a starting point for understanding granular materials, foams, colloids and even glass-forming liquids. Such packings exhibit a jamming transition, known as Point J, with increasing packing fraction. This symposium presents recent work that explores the implications of Point J for systems at nonzero temperature, shear stress, or friction. In this talk, I present results that push beyond zero temperature to explore the connection between Point J and the glass transition. We performed molecular dynamics simulations of several three-dimensional models of glass-forming liquids, and measured the relaxation time from the intermediate scattering function along several trajectories to the glass transition, such as lowering temperature at fixed packing fraction, or raising pressure at fixed temperature. Along each trajectory, we extrapolated the relaxation time using the form $\tau = \exp(A/(T - T_0))$ or $\tau = \exp(A/(p' - p_0))$, depending on whether temperature or pressure was varied, where $p'$ is the contribution to the pressure from repulsive forces, only. Here, $A$, $\alpha$, $T_0$ and $p_0$ are fit parameters. We find that $T_0$ is linear in the repulsive contribution to the pressure, $p'_r$: $T_0 = \nu p'_r$. The fit parameter $\nu$ is approximately $0.035\nu_0 = 0.37\sigma^{-1}$, independent of potential, where $\nu_0$ is the average volume per particle and $\sigma$ is the diameter of the particle. This linear scaling of $T_0$ with $p'$ holds very well at low $p'$, which corresponds to the vicinity of Point J in purely repulsive systems where jamming transition at $T = 0$ exists. This suggests that Point J marks the onset of a nonzero value of the glass transition temperature, $T_0$. Experimental data for glycerol (K. Z. Win and N. Menon, Phys. Rev. E 73, 040501 (2006)) also show that $T_0$ is linear in pressure, with a prefactor of $0.04 \times$ the molecular volume.

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1Supported by DE-FG02-05ER46199 and DE-FG02-03ER46088.

3:06PM L8.00002 Critical Scaling of Shear Viscosity At the Jamming Transition 1, STEPHEN TEITEL, Department of Physics and Astronomy, University of Rochester — I review the assumptions behind a scaling theory of the jamming transition for shear driven non-equilibrium steady states of a granular medium. Scaling predictions are compared against data from numerical simulations for a simple two dimensional model of frictionless soft core interacting disks with overdamped dynamics. Methods are discussed to accurately measure the critical jamming density and the critical exponents describing the jamming transition. Work carried out in collaboration with Peter Olsson, Department of Physics, Umeå University.

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1Supported by DOE grant DE-FG02-06ER46298.
presented.

generalized advection-diffusion and a jump-diffusion scheme. Based on the generalized master equation the corresponding fractional evolution equations are

Walks (CTRWs) in the presence of a prescribed deterministic evolution between the successive transitions. This formulation is exemplified by means of a

JENKO, Max-Planck-Institute for Plasmaphysics, Garching, Germany — We formulate a generalized master equation for a class of Continuous Time Random

Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany, RUDOLF FRIEDRICH, Institute of Theoretical Physics, Muenster, Germany, FRANK

Finally, we also carry out linear stability analysis to validate the results obtained from our algorithm.

Second, we show that, as the number of particles in the system decreases, the magnitude of noise increases and again the Turing patterns form less easily.

Third, we show that, as the system becomes more subdiffusive, the ratio between the two diffusive constants must be higher in order to observe Turing patterns.

to simulate noisy reaction-subdiffusion systems. Using this algorithm, we investigate Turing pattern formation in the Schnakenberg model with subdiffusion.

support from NSF award PHY-0555312 is gratefully acknowledged.

We study an interacting particles system arising from a mapping to the Conserved Kuramoto-Sivashinsky equation. Particles represent vanishing regions of diverging curvature, joined by arcs of a universal parabola; nearest particles are attracted to one another at a rate inversely proportional to their distance, and coalesce upon encounter. Although the model is deterministic, a coarse-grained representation yields a diffusion equation with negative coefficient: the build up of instabilities corresponds to the coalescence events. A preliminary analysis of the model correctly predicts the growth of the typical inter-particle gap with time, but fails to reproduce interesting structure of the probability distribution function for the gap observed in simulations, including a non-trivial power-law at small distances, and a faster than gaussian decay at large distances. At yet an higher level of abstraction, trails of coalescing events may too be viewed as "particles" that propagate ballistically at a speed proportional to the background density, and that annihilate upon encounter.

Support from NSF award PHY-0555312 is gratefully acknowledged.

Work in collaboration with P. Politi (ISC CNR, Italy)

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DANIEL BEN-ARAHAM\textsuperscript{2}, Clarkson University — We study an interacting particles system arising from a mapping to the Conserved Kuramoto-Sivashinsky equation. Particles represent vanishing regions of diverging curvature, joined by arcs of a universal parabola; nearest particles are attracted to one another at a rate inversely proportional to their distance, and coalesce upon encounter. Although the model is deterministic, a coarse-grained representation yields a diffusion equation with negative coefficient: the build up of instabilities corresponds to the coalescence events. A preliminary analysis of the model correctly predicts the growth of the typical inter-particle gap with time, but fails to reproduce interesting structure of the probability distribution function for the gap observed in simulations, including a non-trivial power-law at small distances, and a faster than gaussian decay at large distances. At yet an higher level of abstraction, trails of coalescing events may too be viewed as "particles" that propagate ballistically at a speed proportional to the background density, and that annihilate upon encounter.

S. Maloney, Carnegie Mellon University — No abstract available.

Tuesday, March 17, 2009 2:30PM - 5:30PM –

Session L9 GSNP DBP: Focus Session: Systems Far from Equilibrium II 303

2:30PM L9.00001 A Reacting Particles System arising from the Conserved Kuramoto-Sivashinsky Equation\textsuperscript{1}, DANIEL BEN-ARAHAM\textsuperscript{2}, Clarkson University — We study an interacting particles system arising from a mapping to the Conserved Kuramoto-Sivashinsky equation. Particles represent vanishing regions of diverging curvature, joined by arcs of a universal parabola; nearest particles are attracted to one another at a rate inversely proportional to their distance, and coalesce upon encounter. Although the model is deterministic, a coarse-grained representation yields a diffusion equation with negative coefficient: the build up of instabilities corresponds to the coalescence events. A preliminary analysis of the model correctly predicts the growth of the typical inter-particle gap with time, but fails to reproduce interesting structure of the probability distribution function for the gap observed in simulations, including a non-trivial power-law at small distances, and a faster than gaussian decay at large distances. At yet an higher level of abstraction, trails of coalescing events may too be viewed as "particles" that propagate ballistically at a speed proportional to the background density, and that annihilate upon encounter.

\textsuperscript{1}Support from NSF award PHY-0555312 is gratefully acknowledged.

\textsuperscript{2}Work in collaboration with P. Politi (ISC CNR, Italy)

3:06PM L9.00002 Noisy Transport in Reaction-Diffusion Systems with Quenched Disorder, ANDREW MISSEL, KARIN DAHMEN, University of Illinois, Urbana-Champaign — Reaction-diffusion (RD) models are useful tools for studying a wide variety of natural phenomena. The effects of quenched disorder in the reaction rates on RD models is not completely understood, especially in parameter regimes where internal noise or stochasticity is also important. In this talk, I will discuss an RD model in which both quenched disorder and stochasticity are important. I will show how ideas from the theory of hopping conduction in doped semiconductors and first passage percolation can be used to make predictions for a number of important transport-related features in the model: the infection time, or time needed for the population to traverse the system; the velocity of the front moving through the system; and the dynamic roughening of the coarse-grained front. I will also present the results of simulations of the model that largely confirm these analytical predictions.

3:18PM L9.00003 Monte Carlo simulation and linear stability analysis of Turing pattern formation in noisy reaction-subdiffusion systems, KENG-HWEE CHIAM, A*STAR Institute of High Performance Computing, JIAWEI CHIU, MIT — Subdiffusion is an important physical phenomenon observed in many systems. However, numerical techniques to study it, especially when coupled to noisy reactions, are lacking. In this talk, we develop an efficient Monte Carlo algorithm based on the Gillespie algorithm and the continuous-time random walk to simulate noisy reaction-subdiffusion systems. Using this algorithm, we investigate Turing pattern formation in the Schnakenberg model with subdiffusion. First, we show that, as the system becomes more subdiffusive, the homogeneous state becomes more difficult to destabilize and Turing patterns form less easily. Second, we show that, as the number of particles in the system decreases, the magnitude of noise increases and again the Turing patterns form less easily. Third, we show that, as the system becomes more subdiffusive, the ratio between the two diffusive constants must be higher in order to observe Turing patterns. Finally, we also carry out linear stability analysis to validate the results obtained from our algorithm.

3:30PM L9.00004 Continuous Time Random Walks with Internal Dynamics, STEPHAN EULE, Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany, RUDOLF FRIEDRICH, Institute of Theoretical Physics, Muenster, Germany, FRANK JENKO, Max-Planck-Institute for Plasmaphysics, Garching, Germany — We formulate a generalized master equation for a class of Continuous Time Random Walks (CTRWs) in the presence of a prescribed deterministic evolution between the successive transitions. This formulation is exemplified by means of a generalized advection-diffusion and a jump-diffusion scheme. Based on the generalized master equation the corresponding fractional evolution equations are presented.
3:42PM L9.00005 Unusual finite-size crossover features in driven lattice gases¹. GEORGE L. DAQUILA, UW E C. TAUBER, Virginia Tech — We study the temporal scaling behavior of the autocorrelation function for the asymmetric exclusion process (ASEP) on a ring in one dimension as function of system size and hopping bias. We have performed extensive Monte Carlo simulations using standard and continuous time algorithms to extract the long-time asymptotic scaling behavior for some very large systems. Even for the totally asymmetric exclusion process (TASEP), the effective exponent for the temporal autocorrelation function displays an extremely slow crossover towards the asymptotic value 2/3, with unusual features. For the ASEP, the crossover time grows with increasing backwards hopping rates. In contrast, we observe standard crossover behavior and much shorter crossover times in two- and three-dimensional lattice gases.

¹Research in part supported through NSF DMR-0308548.

3:54PM L9.00006 Contact process with mobile disorder. RONALD DICKMAN — I study scaling properties of the absorbing-state phase transition in the one-dimensional contact process with mobile disorder via numerical simulation and the pair approximation. In this model, the dilution sites are permanently inactive but are free to diffuse, exchanging positions with the other sites, which host a basic contact process. Even though the disorder variables are not quenched, the critical behavior is drastically affected: the critical exponent $\delta$ and the ratio $\beta/\nu$ are found to vary continuously with vacancy concentration and hopping rate. At the critical point, the mean lifetime $\tau$ scales with system size $L$ as $\tau \sim (\ln L)^2$, rather than as a power law; the anomalous scaling of the lifetime is associated with fluctuations in the vacancy density.

4:06PM L9.00007 Fluctuation ratios in reaction-diffusion systems, SVEN DOROSZ, MICHEL PLEIMLING, Virginia Polytechnic Institute and State University — We study fluctuations in diffusion-limited reaction systems driven out of their stationary state. Using a numerically exact method, we investigate fluctuation ratios in various systems which differ by their level of violation of microscopic time reversibility. Studying a quantity that for an equilibrium system is related to the work done to the system, we observe that under certain conditions oscillations appear on top of an exponential behavior of transition fluctuation ratios. We argue that these oscillations encode properties of the probability currents in state space.


4:30PM L9.00009 Stochastic current switching behavior in semiconductor superlattices. STEPHEN TEITSWORTH, HUIDONG XU, Duke University — Numerical simulation results are presented for a discrete drift-diffusion model that describes electronic transport in weakly-coupled semiconductor superlattices under voltage bias and also includes shot noise in the tunneling currents. Sequential resonant tunneling between quantum wells is the primary conduction mechanism and noise terms are treated as delta-correlated in space and time. We study the response of this system to abrupt steps in applied voltage in a range for which the current-voltage characteristics exhibit bistability. The system switches from a metastable state to a stable state with a stochastically varying delay time, a process corresponding to relocation of charge density from one (critical) quantum well to an adjacent one. We find that the mean delay time $\tau$ varies as $\ln \tau \propto V - V_{ch}^{1/2}$ where $V$ and $V_{th}$ denote, respectively, the system voltage and the voltage at the boundary of the bistability range [1]; $\tau$ also depends exponentially on the cross-sectional area of the superlattice. An effective one-dimensional potential energy is constructed for the charge density in the critical quantum well. We find that noise contributions of the quantum wells far from the critical well have a significant effect on the switching process. [1] O. A. Tretyakov and K. A. Matveev, Phys. Rev. B. 71, 165326 (2005).

⁵Supported by NSF grant DMR-0804232.

4:42PM L9.00010 Fluctuation relations in a driven, nonlinear micromechanical torsional oscillator. COREY STAMBAUGH, H.B. CHAN, University of Florida — Fluctuation relations in a periodically driven micromechanical oscillator are investigated. The system is first studied in a linear regime by applying a weak drive. The ratio of the work variance to the mean work is shown to be independent of the driving frequency, consistent with standard fluctuation relations for a steady state system near thermal equilibrium. When a strong drive is applied to the system the response becomes nonlinear and the system displays bistability. The work variance in this nonlinear system, driven far from equilibrium, is predicted to show a strong frequency dependence not seen in the linear case. For such bistable system the total variance has two contributing components. The first component, involving intrastate fluctuations about one stable attractor, is expected to scale with a power law dependence as the system approaches the bifurcation point where the occupied state disappears. The second component of the work variance for interstate fluctuations is shown to have a strong frequency dependence near the kinetic phase transition where the populations of the two states are comparable. The relationship between the work and variance is compared to experimental observations, and to theory.

4:54PM L9.00011 ABSTRACT WITHDRAWN —

5:06PM L9.00012 Work distributions in the T=0 Random Field Ising Model. XAVIER ILLA, Helsinki University of Technology, JOSEP MARIA HUIGUET, EDUARD VIVES, Universitat de Barcelona — The T=0 Random Field Ising Model is a prototype model for the study of collective phenomena in disordered systems. The model can be numerically studied from two different points of view: on the one hand, the exact ground state calculation provides an approach to the equilibrium phase diagram. On the other the use of a local relaxation dynamics based on single spin-flips provides a good framework for the understanding of avalanche dynamics and hysteresis, which is closer to experimental observations. In this sense, the model is a good workbench for the comparison of equilibrium and out-of-equilibrium trajectories. We perform a numerical study of the three-dimensional Random Field Ising Model at T=0. We compare work distributions along metastable trajectories obtained with the single-spin flip dynamics with the distribution of the internal energy change along equilibrium trajectories. The goal is to investigate the possibility of extending the Crooks fluctuation theorem to zero temperature when, instead of the standard ensemble statistics, one considers the ensemble generated by the quenched disorder. We show that a simple extension of Crooks fails close to the disordered induced equilibrium phase transition due to the fact that work and internal energy distributions are very asymmetric.
3:06PM L10.00004 Quasiparticle Gaps and Exciton Coulomb Energies in Si Nanoshells, KIMBERLY FREY, JUAN C. IDROBO, SERDAR OGUZ\textsuperscript{1}, University of Illinois at Chicago, MURILLO L. TIAGO, FERNANDO A. REBOREDO\textsuperscript{2}, Oak Ridge National Laboratory — Quasiparticle gaps and exciton Coulomb energies are calculated in Si nanoshells passivated by H at the inner and outer surfaces. We consider spherical nanoshells with inner radii \( R_1 \) up to 1 nm and outer radii \( R_2 \) up to 1.6 nm. Quasiparticle gaps are calculated using the \( \Delta SCF \) and \( GW \) methods. While the single-band effective mass approximation predicts that the gap should depend only on the thickness \( t = R_2 - R_1 \), we find that first principles calculations that depend on both \( R_1 \) and \( R_2 \). The dependences of the quasiparticle gap on \( R_1 \) and \( R_2 \) are mostly consistent with electrostatics of a charged metallic shell. We also find that the (unscreened) Coulomb energy in Si nanoshells has a somewhat unexpected size dependence at fixed outer radius \( R_2 \). Namely, the exciton Coulomb energy decreases as the nanoshell becomes more confining, contrary to what one would expect from quantum confinement effects. We show that this is a consequence of an increase in the average electron-hole distance, giving rise to reduced exciton Coulomb energies in spite of the reduction in the confining nanoshell volume.

\textsuperscript{1}Supported by DOE Grant No. DE-FG02-03ER15488

\textsuperscript{2}Supported by the Division of Materials Sciences and Engineering BES, U.S. DOE under grant ERKCS77
3:30PM L10.00006 Ab-initio calculations of optical spectra of silicon nanowires, DARIO ROCCA, GIULIA GALLI, University of California, Davis — We present ab-initio calculations of absorption spectra of thin silicon nanowires (1-2 nm in diameter) and compare the results of different techniques. In particular we aim at assessing the ability of time dependent Density Functional Theory (TDDFT) to describe trends in the electronic properties of Si nanowires, by comparing results obtained within TDDFT with those of the Bethe-Salpeter Equation (BSE). We also discuss the numerical accuracy of both TDDFT and BSE calculations and the influence on computed spectra of several numerical parameters entering the calculations.

1Work supported by NSF grant CHE-0802907

3:42PM L10.00007 Photoluminescence from core/multiple-shell GaAs/AlGAs Nanowires, M.A. FICKENSCHER, S.D. PERERA, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, H.J. JOYCE, Y. KIM, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We use photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE) to study the electronic structure of GaAs/AlGaAs core-shell multi-shell NWs. Using Au-catalyst assisted MOCVD, a nominally 2 nm GaAs quantum well tube (QWT) with AlGaAs barriers is formed surrounding a central 50 nm GaAs nanowire core. PL measurements on single nanowires reveal a line at the expected exciton energy for the core and, in addition, several higher energy lines not observed in simple core/shell structures. PLE measurements suggest a coupling of the confined states in the QWT and the core states. A broad PLE response centered at 1.67 eV is suggestive of an AlGaAs shell concentration of approximately 12%. We acknowledge the support of the NSF (0701703 and 0806700) and the Australia Research Foundation.

3:54PM L10.00008 Polarization Dynamics of Twin Free GaAs/AlGaAs Core-Shell Nanowires, S. PERERA, L.M. SMITH, H.E. JACKSON, University of Cincinnati, J.M. YARRISON-RICE, University of Miami, H.J. JOYCE, Y. KIM, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, X. ZHANG, J. ZOU, University of Queensland — We use polarized time-resolved photoluminescence to study exciton dynamics in GaAs/AlGaAs core-shell nanowires (NWs) at 20 K. By pumping the nanowires with lasers polarized parallel and perpendicular to the nanowire, the polarization dynamics reflect the exciton dipole distributions within the nanowires. The NWs were prepared by Au catalyzed MOCVD and excited by a pulsed titanium-sapphire laser at 798 nm. The polarization of the emitted PL was monitored at the exciton emission peak (1.515 eV) as a function of time after excitation by a polarized pulse. The diameter of the nanowire is much larger than the exciton Bohr radius so that the exciton dipoles are degenerate regardless of orientation; thus in thermal equilibrium the density of excitons parallel and perpendicular dipoles should be equal. At low excitation intensities we find that the exciton dipoles are created out of thermal equilibrium, but relax within several hundred picoseconds. At higher excitation powers, the exciton dipoles relax much more rapidly within a time interval. This suggests that exciton dipole relaxation is very sensitive to carrier-carrier scattering. We acknowledge the support of the NSF (0701703 and 0806700) as well as the Australia Research Foundation.

4:06PM L10.00009 Polarization dependent photoluminescence studies of InP nanowires, LEI FANG, XIANWEI ZHAO, FENGYUAN YANG, EZEKIEL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — Control of the polarization anisotropy observed in measurements of single NWs has the potential to enable both fundamental studies of polarization-sensitive electronic states and potential applications in polarization-sensitive photodetectors. This anisotropy is caused by the large dielectric mismatch between the semiconductor nanowire and the environment (air), which suggests that with appropriate dielectric matching it is possible to minimize or eliminate polarization anisotropy. In order to explore this possibility, we measure the polarization dependence of ensemble InP nanowires grown by pulsed laser deposition. The measured polarization response of these ensembles correlates well with the straightforward extension of previous models developed to describe single wire measurements. Further, initial studies involving coating InP nanowires with tantalum oxide, whose dielectric constant (5.76 to 8.41) is close to that of InP (9.61), reduces the polarization anisotropy by 20%. These preliminary results will be presented and proposed strategies for more dramatic suppression will be discussed.

3:40PM L10.00010 Photocurrent spectroscopy of single InP nanowires, A. MAHARJAN, H.E. JACKSON, L.M. SMITH, A. KOGAN, University of Cincinnati, J.M. YARRISON-RICE, Miami University, S. PAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University — We use photocurrent spectroscopy of single InP nanowires at room temperature to study nanowires having either zinc-blende (ZB) or wurtzite(WZ) crystal structures. Photolithography is used to fabricate the Ti/Al metal contact pads separated by ~4 microns on several ZB or WZ InP nanowires. The metal- semiconductor-metal contacts are modeled based on thermionic emission and field emission theory. Analysis of the dark I-V characteristics of these devices determines important intrinsic properties including donor density, barrier heights and electrical conductivity. Current-voltage (I-V) photocurrent curves for a nanowire are obtained by broad illumination of the device from a Ti-Sapphire laser with energies ranging from 1.30 eV to 1.55 eV. The photocurrent at a given bias voltage is plotted as a function of photon energy to determine the band edge of given semiconductor nanowire. The photocurrent drops exponentially below the band edge reflecting Urbach’s rule. We find that the energy band gaps of wurzite and zinc blende nanowires are 1.42 eV and 1.34 eV respectively at room temperature showing that the energy band gap of wurzite structure is about ~80 meV higher than zinc blende structure. Supported by the NSF (# 0701703, # 0806700 and # 0804199) and the Australian Research Foundation.

4:30PM L10.00011 Photoluminescence Study of Type II ZB-WZ InP nanowire homostructures, K. PEMASIRI, M. MONTAZERI, R. GASS, H.E. JACKSON, L.M. SMITH, University of Cincinnati, J.M. YARRISON-RICE, Miami University, S. PAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, X. ZHANG, J. ZOU, University of Queensland — We use CW and time-resolved photoluminescence (TRPL) from single InP nanowires containing both wurzite (WZ) and zincblende (ZB) crystalline phases to study the quantum confinement of excitons in a Type-II homestructure. We observe strong excitation power dependence, with a change in PL emission energy from the ZB edge to the WZ edge confirming the confinement of the electric field within the space charge region due to the applied bias voltage. Photogenerated electrons and holes are collected at forward and reverse biased contacts, respectively. Polarization analysis shows that the photocurrent is maximized for laser excitation polarized perpendicularly to the c-axis of the nanosheet. Supporte by the NSF (#0701703 and #0806700), KIST Research Foundation and KIST.
4:54PM L10.00013 Raman Stress Mapping of Cds Nanosheets, M. MONTAZERI, J.M. YARRISON-RICE, L.M. SMITH, H.E. JACKSON, University of Cincinnati, H. RHO, Y. LEE, Chonbuk National University, Y.J. CHO, J. CHOJ, J.G. PARK, Korea Institute of Science and Technology — We present results of spatially resolved room temperature second order Raman scattering measurements for single ~3 micron wide CdS nanosheets. The sheets, grown by pulsed laser deposition using vapor-phase transport, are uniform in size and shape and exhibit hexagonal wurtzite structure. The orientation of the c-axis is determined by Raman polarization analysis. Spatially-resolved Raman scattering reveals a stress gradient across the nanosheets, with the 2LO phonon energy at the center of nanosheet being higher by ~2 cm\(^{-1}\) with respect to the edges which indicates that nanosheets are relaxed at the edges with a strain gradient toward the center. Support provided by NSF (#0701763 and #0806700), Korea Research Foundation and KIST.

5:06PM L10.00014 Ultrafast spatially-resolved carrier dynamics in single CdSe nanobelts, LARS GUNDLACH, PIOTR PIOTROWIAK, Department of Chemistry, Rutgers University-Newark, 73 Warren St, Newark, NJ, 07102 — A recently constructed Kerr-gated microscope was applied to spatially, temporally, and spectrally resolve the ultrafast non-linear excitation relaxation dynamics in single CdSe nanobelts. Luminescence movies with a 100 fs frame resolution were constructed. The ability to spatially resolve the femtosecond dynamics in a single emitting object gives insights which would be impossible to obtain in an ensemble measurement. By applying the Kerr-gated microscope we are able to monitor the dynamics in a single nanobelt with a sufficient time resolution to reveal the different pathways that compete with the dissociation of multiple excitons. We will show that ensemble averaging methods give results that are complicated because of ensemble inhomogeneities. Indeed, already a different orientation of the nanoparticles with respect to the light-field leads to different dynamic response and difficult to interpret results. The onset of nonlinear behavior and the subsequent dynamics are particularly sensitive to the most subtle inhomogeneities in composition and morphology and hence most difficult to study under the condition of ensemble averaging making time-resolved wide-field fluorescence microscopy a perfect aid in disentangling the complex response.

Tuesday, March 17, 2009 2:30PM - 5:18PM — Session L11 DMP: Focus Session: Transport Properties of Nanostructures III: Molecular Junctions II 305

2:30PM L11.00001 Electron Transport in Single Molecule Junctions: Stability, Electron-Phonon Interactions and Current-Induced Local Heating, N.J. TAO, Arizona State University — Understanding electron transport in a single molecule connected to two electrodes is as basic task in molecular electronics. A widely used approach is to attach the molecule with two linkers that can bind to the electrodes. Thiol is the most studied linker because of its well known capability to bind strongly to metal electrodes, such as Au, although several other linkers, such as isocyanide, amine, pyridine, carbon-carbon and carboxylic acid, have also been used to establish a molecule-electrode contact. It has been concluded that the linkers can play an important or even dominant role in the conductance and other electron transport properties of molecular junctions. Since the molecule-electrode contact is often the weakest link in a molecular junction, an important question that has not yet been well studied is: How stable is a molecular junction due to the finite lifetime of the linker-electrode bond? Another important question is: How hot does a molecular junction get when passing a current through it? In the present work, we investigate the stability and breakdown mechanism of a single molecule covalently attached to two gold electrodes via Au-S bonds. We report on an experimental study of current-induced local heating in single molecules covalently attached to two gold electrodes as a function of applied bias and molecular length. We also discuss the related electron-phonon interactions in single molecule junctions.

3:06PM L11.00002 Electron Transport and Thermoelectricity in Alkanethiol Molecular Junctions, YU-CHANG CHEN, CHUN-LAN MA, DIU NGHIEIM, YU-SHEN LIU, Department of Electrophysics, National Chiao Tung University, Taiwan — We investigate the electron transport properties of alkanethiol molecules in the two- and three-terminal junctions by using first-principles approaches. We observe that novel states around the Fermi levels are introduced in the amino-substituted butanethiol junction. It leads to a sharp increase of the current owing to the resonant tunneling. We also describe a field-theoretic theory combined with first principles approaches to calculate the thermoelectricity. The dependence of the Seebeck coefficient on the biases, gate voltages, and temperatures is systematically investigated. Due to the novel states introduced by the amino-substituted butanethiol junction, the Seebeck coefficient could be easily controlled by using gate voltages and biases. When the temperature in one of the electrodes is set to zero, the Seebeck coefficient could vary pronouncedly with the temperature in the other electrode, and such dependence could be enhanced by varying gate voltages. At finite biases, we also find richer features in the Seebeck coefficient related to the density of states in the vicinity of the left and right Fermi levels.

3:18PM L11.00003 Ab initio transport calculations of molecular wires with electron-phonon couplings, KENJI HIROSE, NEC Corp., NOBUHIKO KOBAYASHI, Univ. of Tsukuba — Understanding of electron transport through nanostructures becomes important with the advancement of fabrication process to construct atomic-scale devices. Due to the drastic change of transport properties by contact conditions to electrodes in local electric fields, first-principles calculation approaches are indispensable to understand and characterize the transport properties of nanometer-scale molecular devices. Here we study the transport properties of molecular wires between metallic electrodes, especially focusing on the effects of contacts to electrodes and of the electron-phonon interactions. We use an ab initio calculation method based on the scattering waves, which are obtained by the recursion-transfer-matrix (RTM) method, combined with non-equilibrium Green's function (NEGF) method including the electron-phonon scatterings. We find that conductance shows exponential behaviors as a function of the length of molecular wires due to tunneling process determined by the HOMO-LUMO energy gap. From the voltage drop behaviors inside the molecular wires, we show that the contact resistances are dominant source for the bias drop and thus are related to local heating. We will present the electron-phonon coupling effects at contact on the inelastic scattering and discuss on the local heating and local temperature, comparing them with those of metallic atomic wires.

3:30PM L11.00004 Transport properties and stability of molecular break junctions, NIKOLAI SERGUEEV, Vanderbilt University, LEONIDAS TSETSERIS, Vanderbilt University, Aristotele University of Thessaloniki, KALMAN VARGA, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory — The electrode-molecule interface in a break junction is known to be crucial to understand its electronic and transport properties. Using first-principles calculations we first probe a comprehensive set of mechanisms responsible for the stability of the prototype junction of a benzene-dithiol (BDT) between gold electrodes. We find that by pulling the electrodes apart the geometry of the molecule depends drastically on the electrode-surface morphology. We next report results of the quantum transport calculations for several stable junction configurations. The calculations are performed using the recently developed technique based on density functional theory and complex absorbing potentials[1]. The molecular junction is treated as a closed system with a set of complex potentials mimicking the source and the drain electrodes. We will present the results of recent experiments on BDT break junctions. We will compare the results with recent experiments on BDT break junctions.

3:42PM L11.00005 Electrical Conductance and Reversible Conductance Switching in Molecular Junctions

BERT DE BOER, Molecular Electronics, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — A technology is demonstrated to fabricate reliable molecular metal-molecule-metal junctions with unprecedented device diameters up to 100 µm. The yield of these molecular junctions is close to unity. Stability investigations have shown a shelf life of years and no deterioration upon cycling. Key ingredients are the use of a conducting polymer layer (PEDOT:PSS) sandwiched between the self-assembled monolayer (SAM) and the top electrode to prevent electrical shorts, and processing in lithographically defined vertical interconnects (vias) to prevent both parasitic currents and interaction between the environment and the SAM [1–3]. Furthermore, a fully functional solid-state molecular electronic switch is manufactured by conventional processing techniques. The molecular switch is based on a monolayer of photochromic diarylethene molecules sandwiched between two electrodes. The monolayer reversibly switches the conductance by more than one order of magnitude between the two conductance states via optical addressing. This bidirectional conductance switch operates as an electronic ON/OFF switch and as a reprogrammable data storage unit that can be optically written and electronically read [4].


The research was financially supported by the Zernike Institute for Advanced Materials, NWO via the VIDI grant, and NanoNed, a national nanotechnology program coordinated by the Dutch Ministry of Economic Affairs.

4:18PM L11.00006 Reversible, mechanically-activated switching in pyridine single molecule junctions

MARIA KAMENETSKA, Columbia University (CU), SU YING QUEK, Lawrence Berkeley National Lab (LBNL), MICHAEL L. STEIGERWALD, CU, HYOUNG JOON CHOI, Yonsei University, STEVEN G. LOUIE, LBNL, MARK S. HYBERTSEN, Brookhaven National Lab, J.B. NEATON, LBNL, LATHA VENKATARAMAN, CU — We measured the conductance of single pyridine-terminated molecules by mechanically forming and breaking Au point contacts with a modified STM in a solution of molecules. Conductance traces recorded while stretching the junction reveal two distinct steps at different conductance, both due to the formation of a single molecule junction between gold electrodes. To better understand the origin of this bi-stable conductance signature, we devise a new method to experimentally determine the distance between the gold electrodes for any given molecular conductance. We find a clear correlation between the level of conductance and the distance between gold electrodes, with the lower conductance corresponding to a molecule fully stretched between the contacts and the higher conductance to a molecule bound at an angle. The dependence of conductance on metal-molecule contact geometry allows us to reversibly switch between conductance states by elongating and compressing the junction.

1. Support: NSF-CHE-0641523 and NYSTAR.

4:30PM L11.00007 First-Principles Studies of Single-Molecule Junctions: Conductance and Mechanically-Controlled Switching

SU YING QUEK, Molecular Foundry, Lawrence Berkeley National Lab, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University, Seoul; STEVEN G. LOUIE, Department of Physics, University of California, California, Berkeley and Lawrence Berkeley National Lab, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics and Center for Transport in Nanostuctures, Columbia University, J.B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab — We explore the conductance of amine- and pyridine-Au single-molecule junctions, in the context of recent experiments, with a density-functional theory (DFT)-based scattering state approach. Using a physically motivated self-energy correction, we compute conductance values in good agreement with experiment, in contrast to DFT values that are too large[1]. We investigate quantitatively conductance trends, and demonstrate, together with experiment, that reversible conductance switching can result from mechanically-induced changes in the metal-molecule contact geometry in pyridine-Au junctions. [1] Quek et al, Nano Lett 7, 3477 (2007)

1. Support: DOE (DE-AC02-05CH11231, DE-AC02-98CH10886), NSF (DMR-0551195, DMR04-39768, CHE-0117752), NYSTAR, NERSC

4:42PM L11.00008 Conductance of Molecular Wires Measured by STM- Break Junction

JONATHAN R. WIDAWSKY, MARIA KAMENETSKA, ADAM C. WHALLEY, JENNIFER E. KLARE, COLIN NUCKOLLS, MARK S. HYBERTSEN, LATHA VENKATARAMAN, Columbia University and CFN, Brookhaven National Laboratory — We present a comparison of the measured conductances of short molecular wires attached to gold electrodes in ambient conditions. The junctions are fabricated using a modified STM to repeatedly form and break Au point contacts, characterized by the quantum of conductance, in a solution of molecules. Specifically, we characterized the conductance of three molecules – 4,4’-diaminoazobenzene, 4,4’-diaminostilbene, and bis-(4-aminophenyl)acetylene – by measuring the voltage bias applied across the electrodes. In order to determine a statistically most probable value of conductance, each measurement is obtained from data sets of approximately 10,000 individual conductance pull-out traces obtained over a few hours. In addition, we measure the conductance of solutions irradiated with ultraviolet light to detect photodesorption of the azobenzene and stilbene from their trans to the cis configurations.


4:54PM L11.00009 Molecular orbital theory of ballistic electron transport through molecules


We gratefully acknowledge financial support provided by NSERC.

1. We gratefully acknowledge financial support provided by NSERC.
Tuesday, March 17, 2009 2:30PM - 5:30PM –
Session L12 DMP DCMP: Focus Session: Photocatalysis and photovoltaic: Excitation, Trapping, and Transport of Charge Carriers at Surfaces and Interfaces

2:30PM L12.00001 Polynuclear Metal Oxide Photocatalysts in Nanoporous Silica Scaffolds for Artificial Photosynthesis, HEINZ FREI, LBNL — No abstract available.

3:06PM L12.00002 Understanding and Controlling Photovoltaic Effects in Complex Oxide Thin Films, STEVEN BYRNES, THOMAS CONRY, SOURAV ROGER BASU, LANE MARTIN, DREW PARAN, VARADA BAL, JOEL W. AGER, R. RAMESH, UC Berkeley and Lawrence Berkeley National Laboratory — Thin-film oxide heterostructures are a promising material system for large-scale photovoltaic energy conversion, as oxides can be cheap, abundant, stable, and highly light-absorbing. As a model system, we have investigated the room-temperature ferroelectric BiFeO$_3$ (BFO). Heteroepitaxial BFO films are grown by both metal-organic chemical vapor deposition (MOCVD) and pulsed laser deposition (PLD), allowing for a wide range of control over thickness, composition, and ferroelectric domain structure. BFO has been measured to have a direct bandgap at 2.6 eV; moreover its bandgap and other material properties can be controlled by alloying and by modification of stoichiometry. In this work, we will demonstrate the photovoltaic properties of BFO thin films (100–1000 nm) grown heteroepitaxially on oxide bottom electrodes with transparent ITO top contacts. Electrical and external quantum efficiency measurements prove that the photovoltaic effect comes from a Schottky barrier between ITO and p-type BFO, but time-dependent and capacitance-voltage measurements show that ferroelectric, ion motion, and/or trap states also play an important role in the electrostatics of the device.

3:18PM L12.00003 Ultrafast Time-Resolved Spectroscopy of Photoinduced Electron Transfer in Novel Photovoltaic Devices, L.M. MIER, Department of Chemistry, The Ohio State University, Columbus, OH 43210-1185, A.R. CARTER, Department of Physics, The Ohio State University, Columbus, OH 43210, T.L. GUSTAFSON, Department of Chemistry, The Ohio State University, Columbus, OH 43210-1185, A.J. EPSTEIN, Departments of Physics and Chemistry, The Ohio State University, Columbus, OH 43210 — We present work toward an understanding of the fundamental photophysics of photoinduced electron transfer between 9-anthracenecarboxylic acid (9-AC) and TiO$_2$ nanoparticles in order to apply the techniques to a novel photovoltaic device. The active layer of a proposed device consist of a broad-spectrum, metal-organic absorbent covalently bound through a carboxylic acid to a nano-porous TiO$_2$ structure. To study the electron transfer, a model compound, 9-AC, is covalently bound to TiO$_2$ nanoparticles. Ultrafast electron transfer from the excited 9-AC to the TiO$_2$ is observed within 50 fs using ultrafast broadband spectroscopy. Further evidence of this transfer is shown from quenching of the fluorescence of the 9-AC with increasing concentrations of TiO$_2$ with no effects on the lifetime of the fluorescence.

3:42PM L12.00005 Interfacial charge dynamics studied by ultrafast electron diffraction, RYAN MURDICK, RAMAKANTALAYAN RAMAN, Michigan State University, YOSHI MURUOKA, Osaka University, RICHARD WORTHATCH, CHONG-YU RUAN, Michigan State University — Of central importance to nanoscale device technology is the role of charge transfer at interfaces. Using ultrafast electron diffraction, which has recently emerged as a new technique in determining transient surface photovoltages with nanometer sensitivity (Murdick et al., PRB 77, 245329, 2008), we investigate the surface charge and space-charge dynamics at the Si/SiO$_2$ interface. By varying the excitation wavelength, fluence, and pulse duration, we explore various pathways inducing electron tunneling through an insulating barrier to reach the surface states. We show that the surface states have relatively long lifetimes (~100 ps), but are rechargeable, thus ideal for serving as a charge pump for interfacial devices. Using the Si/SiO$_2$ platform, we extend this diffractionic potentiometry approach to study nanoparticle charging and molecular transport.

1 This work is supported by NSF through grant no. ECCS-0643420.

2 This work is supported by NSF RII Grant EPS 0554328 with matching support from the WVU Corporation and the WV EPSCoR Office, and by NSF HP GS1280 system at the Pittsburgh Supercomputing Center.

3 Funded by NSF RII Grant EPS 0554328 with matching support from the WVU Corporation and the WV EPSCoR Office, and by NSF HP GS1280 system at the Pittsburgh Supercomputing Center.

4 This work was supported by the Department of Energy under Grant No. DE-FG02-06ER46309 and the ACS Petroleum Research Fund under Grant No. 45982-G10.
3:54PM L12.00006 TiO2 nanowire sensitized by organic dyes for photovoltaic applications: influence of binding groups and molecular dimension

SHENG MENG, EFTHIMIOS KAXIRAS, Harvard University Physics Department — We investigate the electronic couplings including charge separation, injection, and recombination processes between a TiO2 nanowire and a set of organic dye sensitizers, based on the full time-dependent density functional theory treatment of electron excitation and atomic vibrations. For all the cases the highest occupied molecular orbital (HOMO) of dye molecules are found being located in the middle of the TiO2 bandgap and the lowest-unoccupied molecular orbital (LUMO) close to the TiO2 conduction band minimum, leading to enhanced visible light absorption and ultrafast electron injection into the TiO2 conduction band. The influences of the anchoring groups and molecular dimensions to the dye injection dynamics and electron-hole recombination process are discussed.

This work was supported in part by DOE CMSN Grant DE-FG02-05ER46226 and the Harvard University Center for the Environment.

4:06PM L12.00007 Analysis of Quasiparticle Energy Band Shifts Resulting from Introduction of Nitrogen into Titanates

WEI KANG, Center for Functional Nanomaterials, Brookhaven National Laboratory, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Laboratory — Titanium oxides and many titanates, such as rutile (TiO2) and SrTiO3, are promising in photocatalysis for water splitting and photo-degradation of hazardous materials in the environment, although their large band gaps limit utilization of the solar spectrum to the UV region. Experiments show that introduction of nitrogen by various means can significantly affect the band gap. However, catalytic action also depends on individual conduction and valence band alignments. We address these issues by performing theoretical calculations of the energy spectrum for titanium oxides, titanates and various structures introducing nitrogen into the crystals using the GW method. In contrast to density functional theory approaches, the GW method generally leads to energy levels and band gaps that agree well with experiments. We here use this approach to illustrate the mechanism of band shifting in titanates due to the introduction of nitrogen, in particular the differences in correlation effects for nitrogen related energy bands in these materials. This work is supported by the DOE.

4:18PM L12.00008 Nanocrystal-based Dyads for Solar to Electric Energy Conversion

LEI WANG, MINGYAN WU, DAVID WALDECK, University of Pittsburgh — We describe a new project which aims to develop a systematic and modular approach to creating a new generation of Gratzel-inspired solar energy conversion devices with the following novel advantages: the ability to capture the entire available range of solar irradiance by employing sets of linked nanoparticles, fabrication by self-assembly, enhanced robustness, and lowered cost through use of nanostuctured, rather than molecular, charge transfer elements. The project team is designing, creating, and characterizing linked-nanoparticle dyads, which will act as the charge separation "engine" in new generation solar cells. By employing a mixture of dyads it should be possible to efficiently capture the entire solar spectrum. The proposed device architecture has two important advantages over existing solar conversion devices: It can be produced by a self-assembly process. Because of its modularity, each of its components (nanoparticles or organic linker) can be optimized separately.

This work is supported by the U.S. Department of Energy, Solar Energy Utilization Initiative

4:30PM L12.00009 Energy level alignment of zinc tetrphenylporphyrins derivatives adsorbed on wide band gap semiconductor oxides

SYLVIE RANGAN, ROBERT ALLEN BARTYNSKI, ELENA GALOPPINI, Rutgers University — Metalloporphyrins play an essential role in photosynthetic mechanisms and therefore are natural candidates for electron transfer mediator in dye sensitized solar cells (DSSCs). Among the possible metalloporphyrins, the zinc tetrphenylporphyrins (ZnTPP) derivatives have been found to have similar electron injection and charge recombination properties as the important standard ruthenium dye N3 for DSSCs, as well as reasonable performances using TiO2 or ZnO as substrates. We have investigated the electronic structure, energy level alignment, and their changes with altered surface bonding geometries, using a selective functionalization with carboxylic anchoring groups of the meso-phenyl, of functionalized ZnTPP on single crystal TiO2 and ZnO surfaces. Occupied and unoccupied electronic states were determined using direct (ultra-violet and x-ray) photoemission and inverse photoemission in the same ultra-high vacuum analysis chamber. Energy level alignment of the ZnTPP molecular orbitals with respect to the substrates band edges will be compared to the available literature.


CHRISTOPHER MERCHANT, NINA MARKOVIC, Johns Hopkins University — We have studied photocurrent generation in large carbon nanotube (CNT) films using electrodes with different spacings. We observe that the photocurrent depends strongly on the position of illumination, with maximum observed response occurring upon illumination at the electrode edges. The rate of change of the response decays exponentially, with the fastest response occurring for samples with the smallest electrode spacing. We show that the time response is due to charge carrier diffusion in low-mobility CNT films.

4:54PM L12.00011 Efficient photocatalysis at pH7: in-situ formation of a water-splitting cobalt catalyst at electrode interfaces

MATTHEW KANAN, MIT — No abstract available.

Tuesday, March 17, 2009 2:30PM - 5:30PM
Session L13 DCOMP: Computational Methods: Quantum Monte Carlo 309

2:30PM L13.00001 ABSTRACT WITHDRAWN

2:42PM L13.00002 PIMC Simulation of Thermal Dissociation of Dipositronium

MINGYAN WU, DAVID WALDECK, University of Pittsburgh — We describe a new project which aims to develop a systematic and modular approach to creating a new generation of Gratzel-inspired solar energy conversion devices with the following novel advantages: the ability to capture the entire available range of solar irradiance by employing sets of linked nanoparticles, fabrication by self-assembly, enhanced robustness, and lowered cost through use of nanostuctured, rather than molecular, charge transfer elements. The project team is designing, creating, and characterizing linked-nanoparticle dyads, which will act as the charge separation "engine" in new generation solar cells. By employing a mixture of dyads it should be possible to efficiently capture the entire solar spectrum. The proposed device architecture has two important advantages over existing solar conversion devices: It can be produced by a self-assembly process. Because of its modularity, each of its components (nanoparticles or organic linker) can be optimized separately.

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also serve as a guide for the hybrid DFT itself. For instance, it provides hints how the weight is changed/screened when a crystal is compressed.

The weight of the exact exchange term optimized in this way can serve as a variational parameter that is optimized with the density-functional-based orbitals. Presented possibilities to improve variational freedom of Slater-Jastrow trial wave function by using one-body orbitals from the hybrid density-functional theory (DFT) to construct its determinantal Slater part. The weight of the exact exchange term in the hybrid DFT functional serves as a variational parameter that is optimized with respect to the total energy calculated within the fixed-node diffusion Monte Carlo method. This approach is certainly less powerful than direct optimization of one-body orbitals within a basis-set expansion, but its modest computational requirements make it suitable for large-scale simulations of solids. Presented method will be illustrated on several materials with emphasis on transition-metal compounds. The weight functional terms in the variational Monte Carlo calculations compared to those given by the density-functional-based orbitals. Advantages of using the optimized orbitals in the diffusion Monte Carlo calculations are also discussed.

We explore possibilities to improve variational freedom of Slater-Jastrow trial wave function by using one-body orbitals from the hybrid density-functional theory (DFT) to construct its determinantal Slater part. We analyze the fixed-node errors for a diverse set of atoms and molecules. In some cases, our simple wavefunctions have almost the exact atomic total energies in the variational Monte Carlo calculations compared to those given by the density-functional-based orbitals. Advantages of using the optimized orbitals in the diffusion Monte Carlo calculations are also discussed.

Improved Algorithm for Calculating Observables in Diffusion and Reptation Monte Carlo. Unlike previous attempts [1], our technique assumes no knowledge about derivatives of the trial or exact ground state wavefunction with respect to the perturbation. We will outline the derivation of the operator and show examples for DMC by comparing to forward walking, and within RMC by showing faster convergence to the unbiased, ground state observable. [2]Assaraf and Caffarel, J. Chem. Phys. 119, 10536 (2003).

Analysis of fixed-nodes errors in quantum Monte Carlo calculations of atoms and molecules, SHUMING HU, KEVIN RASCH, MINYI ZHU, MICHAL BAJDICH, LUBOS MITAS. Center for High Performance Simulation, Department of Physics, North Carolina State University — The accuracy of fixed-node QMC calculation is determined by the fermion nodes of the trial wavefunction. We analyze the fixed-node errors for a diverse set of atoms and molecules. In some cases, our simple wavefunctions have almost the exact nodes. But in other cases, it is very difficult to find the exact nodes even with wavefunctions of correlated many-body forms, such as extensive multi-reference expansions, pairing and backflow. We try to elucidate the impact of the size and extent of the basis sets as one of the factors influencing fixed-node biases. The testing systems also include transition metal atoms with all-electron and Ne-core pseudopotential calculations.

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Geometry of fermion nodes and its impact on many-body effects in quantum Monte Carlo, LUBOS MITAS, North Carolina State University — Fermion nodes, which are zero sets of stationary fermionic many-body wavefunctions, play an important role in quantum Monte Carlo calculations. In the diffusion Monte Carlo method the so-called fixed-node approximation allows us to avoid well-known inefficiencies of the fermion sign problem and to use the method for large systems. Besides this practical importance fermion nodes are also related to spectral properties of second order differential operators and to several physical effects and quantities. In order to understand these relationships, we study fermion nodal hypersurfaces, both their topologies and shapes, as determined by wavefunctions built from different types of correlations such as pairing orbitals and backflow many-body coordinates. We analyze the impact of particle interactions on the changes of nodal topologies and the conditions under which such changes can occur. We investigate impact of nodal topologies on properties of wavefunctions with periodic boundary conditions as well as relationship of the nodal surfaces to kinetic energy and some other quantities. We further attempt to elucidate the nodal properties on examples of exactly solvable models.

Hybrid DFT orbitals as a means of reduction of fixed-node errors in diffusion Monte Carlo simulations, JINDRICH KOLORENC, SHUMING HU, LUBOS MITAS, North Carolina State University — We explore possibilities to improve variational freedom of Slater-Jastrow trial wave function by using one-body orbitals from the hybrid density-functional theory (DFT) to construct its determinantal Slater part. Weight of the exact exchange term in the hybrid DFT functional serves as a variational parameter that is optimized with respect to the total energy calculated within the fixed-node diffusion Monte Carlo method. This approach is certainly less powerful than direct optimization of one-body orbitals within a basis-set expansion, but its modest computational requirements make it suitable for large-scale simulations of solids. Presented method will be illustrated on several materials with emphasis on transition-metal compounds. The weight of the exact exchange term optimized in this way can also serve as a guide for the hybrid DFT itself. For instance, it provides hints how the weight is changed/screened when a crystal is compressed.

Geometry optimization using Quantum Monte Carlo, LUCAS WAGNER, JEFFREY GROSSMAN, University of California, Berkeley — There are many molecular and solid systems where correlation effects need to be treated very accurately to obtain correct geometries. Current density functionals often do not perform sufficiently well in excited states, weak-binding, and transition-metal oxide systems. Quantum Monte Carlo (QMC) offers very accurate total energies due to explicit treatment of electron correlation, but its stochastic nature makes precise geometry optimization challenging. We present a method that uses noisy total energies to perform a stochastic series of line minimizations. This method is efficient for multiple degrees of freedom and is effective in both the excited state and when the trial function is relatively poor—two regimes in which forces in QMC have not been developed. Details of the approach will be presented as well as a number of applications.
4:18PM L13.00010 Quantum Monte Carlo calculations of the energy-level alignment at organic-inorganic hybrid interfaces†, ZHICANG WU, YOSUKE KANAI, JEFFREY GROSSMAN, University of California at Berkeley — Understanding interface properties of nano- and hybrid-composite materials is of critical importance for fostering technological advancements. While the density functional theory (DFT) continues to be an important method for investigating opto-electronic and excitation properties of materials, the DFT calculations in some cases fail to provide an accurate description. One such difficult case is computing the energy-level alignment at a hybrid interface, composed of two distinct materials with very different electronic characteristics. In this work we present a quantum Monte Carlo approach to correct the Kohn-Sham (KS) level alignment, and we demonstrate this approach for hybrid interfaces between the silicon (001) surface and several organic molecules. Our calculations show that for some molecules there is a qualitative difference with the DFT-KS level alignment, completely changing the character of the heterojunctions formed. We will discuss its implication for understanding the opto-electronic behaviors of hybrid interfaces, along with some computational/theoretical challenges in extending this approach further.

†This work was supported by the National Science Foundation (NSF) by University of California at Berkeley under Grant No. 0425914.

4:30PM L13.00011 QMC Study of Optical Switching of Azobenzene Molecule†, RENE DERIAN, MATUS DUBECKY, Inst. of Phys., Slovak Academy of Sciences, Bratislava, Slovakia, LUBOS MITAS, Dept. of Phys., NCSU, Raleigh, IVAN STICH, Inst. of Phys., Slovak Academy of Sciences, Bratislava, Slovakia — Optical Switching of photochromic azobenzene (AB) molecule via first excited singlet-state is studied. AB features two photoswitchable conformations, cis and trans with very different geometries and properties. Using QMC techniques we compute excitation/exoexcitation ground-state — first singlet-excitestate spectra of AB. By a careful QMC optimization of the ground/excited-state wave functions with up to 500 determinants chemical accuracy is obtained for the cis and trans conformers. Our QMC results are significantly superior to DFT results with proper spin symmetry (ROKS) and surpass also the available standard quantum chemistry results such as CAS SCF. These results open up the possibility of simulation of anchored AB opto-mechanical switches.

†Work supported by APVV (APVV-0091-07, LPP-0252-07).

4:42PM L13.00012 Multideterminant quantum Monte Carlo calculations of benzene dimers†, RICHARD G. HENNIG, KATHLEEN A. SCHWARZ, Cornell University, Department of Materials Science and Engineering, CYRUS UMIRIGAR, Cornell University, Department of Physics, JULIEN TOULOUSE, Université Pierre et Marie Curie, France — Benzene dimers represent the prototypical system for weak π-π interactions that determine the bonding for various organic materials and carbon nanostructures. Several previous studies using coupled-cluster and quantum Monte Carlo methods have determined the binding energy of parallel, perpendicular and parallel-shifted configurations of the benzene dimer. Here we present multi-determinant variational and diffusion Monte Carlo calculations for the various benzene dimer configurations. The total energy of the benzene dimers depends strongly on basis set size, orbital coefficients and number of determinants in the trial wave function. The binding energy converges faster than the total energy with basis set size and number of determinants due to partial cancellation of errors. While orbital optimization lowers the total energy, the large number of orbital parameters and hence large computational cost limits orbital optimizations to wave functions with small basis sets and small numbers of determinants. In comparison the optimization of the Jastrow and determinant coefficients can efficiently converge the energy of benzene dimers and enables accurate predictions of the binding energies.

†Funded by the DOE petascale initiative.

4:54PM L13.00013 A Quantum Monte Carlo investigation of dispersion interactions in graphite†, LEONARDO SPANU, UC Davis Chemistry Department, Davis CA, GIULIA GALLI, UC Davis, Chemistry Department, Davis CA, SANDRO SORELLA, SISSA-ISAS, Trieste Italy — We present a series of Quantum Monte Carlo (QMC) calculations of graphite, aimed at describing on the same footing the strong C-C covalent bonds and the weaker interlayer interactions. In particular, we carried out calculations of binding energies, bond lengths and compressibility by using the Variational Monte Carlo and Lattice Regularized Diffusion Monte Carlo techniques [1]. We use as a variational ansatz the Jastrow Antisymmetrized Wave function, including a pairing determinant and a Jastrow correlation factor [2]. Our results allow for a detailed analysis of dispersion forces between graphite layers, including their behavior at long distances, and yield a quantitative estimate of the layer binding energy.


Work supported by DOE/SciDAC DE-FC02-06ER25794

5:06PM L13.00014 Auxiliary-Field Quantum Monte Carlo Studies of Pressure-Induced Phase Transitions in Silicon and MnO†, WIRAWAN PURWANTO, HENRY KRAKAUER, ERIC WALTER, SHIWEI ZHANG, College of William and Mary — Accurate theoretical predictions across structural phase transitions are challenging, as they typically involve different electronic structures on the two sides of the transition. We use the phaseless auxiliary-field quantum Monte Carlo (AFQMC) method—which yields accurate many-body wave functions by means of importance sampled random walks in the space of Slater determinants—to calculate the equation of state near two phase transitions: in Si, from the diamond to metallic β-tin transition at ~ 11 GPa; and in MnO, the volume and magnetic moment collapse at ~ 100 GPa. The Si phase transition serves as a test case to study the accuracy of the AFQMC method; the calculated transition pressure is in good agreement with the experiment. Applications to the MnO phase transition will then be presented.

†Supported by DOE (CMSN and QMC EndStation), ONR, NSF, and ARO. Calculations were performed at NCCS Jaguar

5:18PM L13.00015 A Quantum Monte Carlo Study of Molecular Titanium Dihydride†, TODD D. BEAUDET, JEONGNIM KIM, KENNETH ESLER, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — Recently there has been interest in the possibility of reversibly storing molecular hydrogen on titanium decorated carbon-nanostructures. The possibility of storing molecular hydrogen on titanium decorated carbon nanostructures is of critical importance for fostering technological advancements. While the density functional theory (DFT) continues to be an important method for investigating opto-electronic and excitation properties of materials, the DFT calculations in some cases fail to provide an accurate description. One such difficult case is computing the energy-level alignment at a hybrid interface, composed of two distinct materials with very different electronic characteristics. In this work we present a quantum Monte Carlo approach to correct the Kohn-Sham (KS) level alignment, and we demonstrate this approach for hybrid interfaces between the silicon (001) surface and several organic molecules. Our calculations show that for some molecules there is a qualitative difference with the DFT-KS level alignment, completely changing the character of the heterojunctions formed. We will discuss its implication for understanding the opto-electronic behaviors of hybrid interfaces, along with some computational/theoretical challenges in extending this approach further.

†Supported by DOE (CMSN and QMC EndStation), ONR, NSF, and ARO. Calculations were performed at NCCS Jaguar.
2:30PM L14.00001 The equilibrium colloidal crystal/colloidal liquid interface, ERIC R. WEEKS, JESSICA HERNANDEZ-GUZMAN, Physics Dept., Emory University — We use confocal microscopy to study an equilibrated crystal-liquid interface in a colloidal suspension. The surface shows spatial fluctuations due to capillary waves. Local measurements of the structure and dynamics near the rough surface reveal that the intrinsic surface, while meandering in space, is locally sharply defined. Examining different quantities finds slightly different widths of this intrinsic surface.

2:42PM L14.00002 Janus particles at the liquid-liquid interface, QIAN CHEN, STEPHEN ANTHONY, STEVE GRANICK, University of Illinois Urbana Champaign — Dipolar Janus particles (negatively charged on one side, positively charged on the other), deposited on PDMS droplets in water, are studied in real time by fluorescence and phase contrast microscopy. Crystals form, under some conditions with long-range hexagonal order, but this self-assembled structure depends strongly on particle size and ionic strength of the water phase. Their provocative translational and rotational dynamics is studied using single-particle tracking.

2:54PM L14.00003 Short-time self-diffusion of nearly hard spheres at an oil-water interface, PENGER TONG, YUAN PENG, WEI CHEN, Department of Physics, Hong Kong University of Science and Technology, THOMAS FISCHER, Institute of Experimental Physics V, University of Bayreuth, DAVID WEITZ, Department of Physics and School of Engineering and Applied Sciences, Harvard University — Optical microscopy and multi-particle tracking are used to study hydrodynamic interactions of monodisperse polymethylmethacrylate (PMMA) spheres at a decal-win-water interface. The short-time self-diffusion coefficient measured at low surface coverage has the form, \( D_S^2(n) = \alpha D_0 (1 - \beta n) \), where \( n \) is the area fraction occupied by the particles and \( D_0 \) is the Stokes-Einstein diffusion coefficient in the bulk suspension of PMMA spheres in decal. The measured values of \( \alpha \) are found to be in good agreement with the numerical calculation for the drag coefficient of interfacial particles. The measured values of \( \beta \) differ from that obtained for bulk suspensions, indicating that hydrodynamic interactions between the particles have interesting new features at the interface.

3:06PM L14.00004 Observing the three-dimensional motion of colloids at an oil-water interface, RYAN MCGORTY, DAVID KAZ, Harvard University, SHANKAR GHOSH, Tata Institute of Fundamental Research, V.N. MANOHRAN, Harvard University — Our experimental system allows us to place micron-sized colloids at a flat oil-water interface. Using digital holographic microscopy we track the motion of particles at the interface in all three dimensions. Of particular interest is the out-of-plane motion of an adsorbed particle. I will present data of such motion and what it reveals regarding the energy and length scales of a particle attached to an interface. Introducing a laser tweezer and customized colloids (such as core-shell particles) into our experiment allows us to further investigate this system.

3:18PM L14.00005 Self-assembled Capillary Arrows, JEAN-CHRISTOPHE LOUDET, BERNARD POULIGNY, Centre de Recherche Paul Pascal, CNRS 115 avenue A. Schweitzer 33600 Pessac, France — Anisotropic particles adsorbed at a water-air interface are known to aggregate due to capillary interactions. We show that the packing configuration of a pair of prolate ellipsoids critically depends on their relative size and/or aspect ratio mismatch. While identical particles simply pack side-by-side, particles of slightly different sizes are observed to systematically self-assemble into characteristic arrows, i.e. with a finite angle between their axes. The occurrence of such arrows cannot be explained within the far-field approximation of interacting polar quadrupoles. A numerical analysis is worked out which allows us to explore the near-field characteristics of the capillary interaction. Results clearly show the destabilization of the side-by-side configuration due to a size mismatch, in agreement with experimental observations.

3:30PM L14.00006 Impact of Surfactant Sorption Kinetics on Microscale Tipstreaming, WINGKI LEE, LYNN WALKER, SHELLEY ANNA, Carnegie Mellon University — A microfluidic flow focusing system has been used to synthesize submicron sized droplets via a thread formation mode of drop breakup. This process utilizes the interaction of fluid motion and surfactant transport to draw out a thin thread, which then fragments into a stream of tiny droplets whose sizes are orders of magnitude smaller than the size of the device. In this work, we use a homologous series of C\(_n\)E\(_S\) (\( n = 10, 12 \) and 14) surfactants to probe the impact of surfactant sorption kinetics on this process. To characterize the effects of these surfactants on the thread formation process, we measure the relevant timescales for the formation of a cone-like interface, the drawing and disintegration of a fine thread, and the period with which the process repeats. We then relate these timescales to the characteristic timescales for transport of surfactants to the oil-water interface. These measurements and simple scaling analyses suggest ways to extend the thread length and optimize the overall yield of submicron droplets.

3:42PM L14.00007 Network Formation at the Air-Water Interface, ALINE MILLER, MARIA SIMON SAENZ DE SAMANIEGO, University of Manchester — A series of dicarboxylic end functionalised peptides have been designed to form beta-sheet rich monolayers at the air-water interface and their structure, rheological properties and ability to polymerize in response to UV light have been studied using a Langmuir trough and dilatational rheology. Surface pressure-area isotherms as well as compression-expansion cycles reveal all our peptide monolayers organise into the three distinct organisational states typically observed for surfactants at the air-water interface: gaseous (G), liquid expanded (LE) and liquid condensed (LC) and the limiting area per molecule suggests the alternating amphiphilic structure of the peptide causes the molecule to orient with its long axes parallel to the air-water interface. The presence of the dicarboxylic group enhances surface activity and stability over time. Here we will discuss how peptide sequence, UV exposure strength and time, as well as peptide concentration (and hence organisation) influence the kinetics of network formation, and the morphology and mechanical properties of the final network formed.

3:54PM L14.00008 Kinetically Controlled Adsorption to Freshly Formed Interfaces, NICOLAS ALVAREZ, Chem. Eng. Dept., LYNN WALKER, Chem. Eng. Dept., SHELLEY ANNA, Mech. Eng. Dept., Carnegie Mellon University — The coefficients of diffusion, adsorption, and desorption are fundamental properties of surfactant molecules and should be independent of the nature in which they are applied. However, the approaches currently used to obtain these parameters are highly context dependent and can lead to unphysical trends such as a concentration dependent diffusion coefficient and large mismatches between predicted and observed dynamic behavior. In pendant drop studies one is restricted to diffusion or mixed controlled adsorption at small concentrations, but in reality to get at the kinetic coefficients it would be more advantageous to probe the kinetic controlled regime. Recently it was shown that a characteristic length scale, \( R_{D-K} \), governs the transition from diffusion controlled adsorption to kinetically controlled adsorption for spherical interfaces. If the spherical interface has a radius smaller than \( R_{D-K} \) the adsorption process is kinetically limited. This paper uses a micro-tensiometer to probe the adsorption dynamics to micron diameter spherical interfaces to test the transition from diffusion limited to kinetic limited adsorption. Using this method we measure kinetic adsorption constants directly. We also describe a new timescale for diffusion, which better describes the adsorption of surfactants onto spherical interfaces.

\(^{1}\)Work supported by the Research Grants Council of Hong Kong SAR.

\(^{2}\)This research was supported by the National Science Foundation Grants Nos. CBET-0608864 and CBET-0730727. Acknowledgement is made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.
Structures formed by colloidal particles on a droplet at small particle number. Jerome Fung, Ryan J. McGorty, Harvard University, Dept. of Physics, Vinothan M. Manoharan, Harvard University, Dept. of Physics and SEAS — We discuss 3D imaging studies of the self-assembled structures formed by small numbers (∼10) of micron-sized polymethylmethacrylate (PMMA) colloids pinned to the surface of a ∼10 micron oil droplet in an aqueous solution. In the low N limit, these structures are governed by the interactions between the constituent colloidal particles on a given droplet. We prepare these droplets using a capillary microfluidic device. Since the droplets are not density matched to the continuous phase, we study them with a time-averaged zero gravity apparatus, based on a rotary stage. Specifically, we image the 3D structures formed by the colloidal particles on the droplets using digital holographic microscopy (DHM). DHM records the 2D interference patterns, or holograms, formed by light scattered from the colloidal particles and unscattered light. Subsequent analysis of the holograms, based on the Lorenz-Mie solution for light scattering by spheres, allows us to determine the 3D particle positions with time resolution limited by the camera frame rate.

Interfacial rheology in complex flow. Jeffrey Martin, Steven Hudson, National Institute of Standards and Technology — Multiphase liquid systems are omnipresent in and essential to everyday life, e.g. foods, pharmaceutics, cosmetics, paints, oil recovery, etc. The morphology and stability of such systems depend on dynamic interfacial properties and processes. Typical methods utilized to measure such interfacial properties often employ drops that are much larger and flows that are much simpler than those encountered in typical processing applications. A microfluidic approach is utilized to measure dynamic structure and kinetics in multiphase systems with drop sizes comparable to those encountered in applications and flow complexity that is easily adjustable. The internal circulation and deformation of an aqueous droplet in clear mineral oil is measured using particle tracers and a detailed shape analysis, which is capable of measuring sub-micron deviations in drop shape. Deformation dynamics, detailed drop shape, interfacial tension, and internal circulation patterns and velocities are measured in Poiseuille and transient elongational flows. Flow kinematics are adjusted by varying the microchannel geometry, relative drop size, and drop height. The effects of confinement on interfacial dynamics and circulation patterns and velocities are also explored.

Reverse coffee-ring effect. Byung Mook Weon, Lei Xu, Department of Physics, University of Pennsylvania Amherst, T. Prisk, J. Zhou, A. Dinsmore — We measure the contact forces at the bottom of a container of frictionless liquid droplets as a function of compression and of distance to the container wall. Glass cylinders are used to contain 20-micron-radius droplets of silicon oil; Brownian motion is not significant for this size. Reflection interference contrast microscopy is used since we are particularly interested in contacts with the bottom surface. By looking at the Newton’s ring interference pattern, we measure the deformation of each droplet, which arises from gravity and pressure from the whole pile transmitted through droplet contacts. We also measure the radius of each droplet and thereby obtain the vertical contact force. We vary the pile height to change the compressive stress and then measure the corresponding forces, probability distributions, and correlations of rearrangements. The results elucidate the roles that friction and confining walls play in granular systems and also shed light on force chains in bulk of the material.

Sticking colloids to liquid-liquid interfaces one by one. David Kaz, Ryan McGorty, Harvard University, Shankar Ghosh, Vinothan Manoharan, Harvard University — We investigate the dynamics of placing individual colloidal particles (~2 microns) onto a flat oil-water interface using optical tweezers. By monitoring the strength and position of the trap, we are able to measure the forces acting on a particle as it encounters the liquid-liquid interface. Digital holographic microscopy affords us three dimensional position information at high frame rates (> 500fps), allowing us to probe short timescale behavior. We vary parameters such as particle surface chemistry, dissolved ion concentration, and pH in order to pursue questions about the nature of interface penetration dynamics.

Controlled Crystal Growth and Solid-Liquid Interface in temperature-sensitive colloidal systems. Duc Nguyen, University of Amsterdam, The Netherlands, Zhbing Hu, University of North Texas, Peter Schall, University of Amsterdam, The Netherlands — We use temperature-sensitive colloidal NIPA systems to study crystal growth at the “atomic scale”. By applying a temperature gradient we are able to control the growth of large colloidal single crystals. We visualize the nucleation of these crystals and solidification at the crystal-liquid interface in three dimensions by using confocal microscopy. Trajectories of particles on both the crystal and liquid side of an advancing interface are determined. These elucidate the mechanism of particle assembly at the interface of a growing crystal. At later stages of crystal growth, the interface becomes stationary, and we use the fluctuations of the stationary interface to determine the interface stiffness. Our data suggests a strong anisotropy of the interface tension. These microscopic observations provide unique insight into the mechanism of solidification.

A Surface Plasmon Resonance Investigation of How Water Meets a Hydrophobic Surface. Adele Poynor, Allegheny College, Physics Department. Corey Shemelya — By definition hydrophobic substances hate water. Water placed on a hydrophobic surface will form a droplet in order to minimize its contact area. What happens when water is forced into contact with a hydrophobic surface? One theory is that an ultra-thin low- density region forms near the surface. We have employed the surface-sensitive, quantum-optical technique of Surface Plasmon Resonance (SPR) to verify the existence of this region at the boundary.

2:30PM L15.00001 Thermal Convection in the Presence of Internal Heating. Gabriel Seiden, Stephan Weiss, Eberhard Bodenschatz, Max Planck Institute for Dynamics and Self-Organization — Thermal convection in the presence of internal heat sources is an important mechanism of heat transport in geophysics, particularly in planetary mantle convection. Carefully controlled laboratory studies of this mechanism are, however, scarce. We present experimental results on the effect of internal heating on Rayleigh-Bénard convection, where the heat sources are induced by IR absorption. The results are compared with available theoretical predictions.
2:42PM L15.00002 Chaotic three particle dynamics in a viscous liquid filled rotating drum . JAMES E. DAVIDHEISER, ERIC R. WEEKS, PHIL SEGRE, Physics Dept., Emory University — We conduct experiments to study the motions of three heavy spheres moving within a viscous liquid filled rotating cylindrical drum. Numerous works, in other geometries, demonstrated that assemblies of non-Brownian particles in viscous liquids have the potential to exhibit chaotic motion. We find that as the drum rotation rate ω is varied, there are several distinct periodic states as well as fully chaotic states. We track the motion of the spheres using a digital camera and custom particle tracking software. From our data, we characterize the chaotic trajectories as ω is varied.

2:54PM L15.00003 Chaotic Dynamics of an Elastically Bouncing Dumbbell . COLIN REES, SCOTT FRANKLIN, Rochester Institute of Technology — The dynamics of an elastically bouncing dumbbell is analogous to that of a ball bouncing on a sinusoidally deforming surface with an important exception: the dumbbell’s angle, analogous to the surface’s oscillation frequency, changes with each bounce, making the subsequent motion significantly more complicated. We investigate this dynamical system over a range of aspect ratios and initial energy, finding periodic, quasi-periodic and chaotic motions. As the initial energy is increased, the dumbbell can flip over and tumble. We find for large aspect ratios, however, narrow bands of energies well above this minimum where tumbling suddenly ceases. Because energy is conserved, the dynamics of a bounce are uniquely determined by the angle and angular velocity. The Lyapunov exponents of paths in this two dimensional phase space can be calculated, with the hope of identifying periodic islands within the chaotic sea. Finally, for certain parameters, the angle at each collision moves from its initial value in a subdiffusive manner, and we determine the characteristic exponents.

3:06PM L15.00004 ABSTRACT WITHDRAWN —

3:18PM L15.00005 Fixed point of a renormalization group approach for oscillator synchronization. TONY LEE, GIL REFAEL, MICHAEL CROSS, OLEG KOGAN, Department of Physics, California Institute of Technology. JEFFREY ROGERS, Control and Dynamical Systems, California Institute of Technology — We apply a recently developed renormalization group method to a 1-dimensional chain of phase-coupled oscillators in the regime of weak randomness. The RG predicts how oscillators with randomly distributed frequencies and couplings form frequency-synchronized clusters. Although the RG was originally intended for strong randomness (distributions with long tails), we find good agreement with numerical simulations even in the regime of weak randomness. We also show analytically and numerically the existence of a stable fixed point in the functional RG space. At late stages of the RG, there is a universal approach to the fixed point regardless of the initial distributions of frequency and coupling.

3:30PM L15.00006 Cell refinement and growing misorientations from a continuum dislocation density theory . YONG CHEN, WOOSONG CHOI, STEFANOS PAPANIKOLAOU, JAMES P. SETHNA, Laboratory of Atomic and Solid State Physics, Cornell University, SURACHATE LIMKUMNERD, Physics Department, Chulalongkorn University, Bankok, Thailand — At low temperatures, climb-free plastic behavior of BZ gels through mechanical deformations opens up the possibility of using these materials in novel chemo-mechanical sensors.

3:42PM L15.00007 Dynamic self-assembly in far-from-equilibrium magnetic granular ensembles at the liquid/liquid interface . ALEXEY SNEZHKO, IGOR ARANSON, Argonne National Laboratory — Magnetic particles suspended over an interface of two immiscible liquids and energized by a vertical alternating magnetic fields give rise to novel dynamic self-assembled structures (“pulsating magnetic stars,” “clams”) which are not accessible at the liquid/air interface. These novel structures is attributed to the interplay between surface waves, generated at the liquid/liquid interface by the collective response of magnetic microparticles to the alternating magnetic field, and hydrodynamic fields induced in the boundary layers of both liquids forming the interface. We show that while the onset of the dynamic self-assembly is controlled by the external driving magnetic field parameter the viscosity of the liquids forming the interface plays an essential role. Transition between different self-assembled structures with the parameters of the external excitations is observed.

3:54PM L15.00008 Investigation on dynamics of colloidal particles with optically-controlled electrode patterns1 . Kwan HyOung Kang, HyunJin Park, Horim Lee, Jiwoo Hong, Pohang Univ. Sci. and Tech. — We investigated the dynamics of colloidal particles under ac electric fields. We used an optoelectronic substrate in which the conductivity of substrate can be changed optically. The shape of electrode pattern thus can be changed freely by controlling the optical pattern which is produced by a conventional projector. Interaction between particles showed a various patterns depending on applied electrical frequency, and rich dynamic characters are captured by dynamically changing the electrode pattern. Particle behaviors are in general governed by the balance between the dielectrophoresis and induced charge electroosmosis.

4:06PM L15.00009 Memories in paste: their applications to control crack patterns . AKIO NAKAHARA, YOUSUKE MATSUO, Nihon University — We experimentally find that a paste, i.e., a densely packed colloidal suspension with plasticity, has memories of external mechanical fields it suffered, such as flow and vibration. These memories are sustained as microscopically anisotropic network structures of colloidal particles. By drying these pastes, we find that the memories in pastes can be visualized as macroscopically anisotropic crack patterns. By using the memory effects of paste, we can imprint flow and vibration patterns into pastes to produce various crack patterns, such as lamellar, radial, ring, spiral, and so on [1]. [1] Physics Today 60 (2007), no. 9, p. 116.

4:18PM L15.00010 Controlling chemical oscillations in heterogeneous BZ gels via mechanical strain . VICTOR YASHIN, Chemical Engineering Department, University of Pittsburgh, KRYSNTYN J. VAN VLIES, Department of Materials Science and Engineering, Massachusetts Institute of Technology, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — We performed theoretical and computational studies to determine the effect of an applied mechanical strain on the dynamic behavior of heterogeneous polymer gels undergoing the oscillatory Belousov-Zhabotinsky (BZ) reaction. In these gels, the catalyst for the reaction is localized in specific patches within the polymer network and the BZ reaction only occurs within these BZ patches. We focused on a 1D model for the system, and considered two scenarios, in which the BZ reaction did or did not affect the degree of swelling within the gel. For gels having one and two BZ patches, we found that a longitudinal strain could induce transitions between the oscillatory and steady state regimes. For certain values of the BZ stoichiometric parameter f, these transitions could exhibit a hysteresis. In systems having two oscillating BZ patches, a strain could switch between the in-phase and out-of-phase synchronization of the oscillations. The ability to alter the dynamic behavior of BZ gels through mechanical deformations opens up the possibility of using these materials in novel chemo-mechanical sensors.
of a quantum phase transition where \( \Omega \) is possible, by choosing the parameters of the system appropriately, to produce an interacting 1D bose gas with sharp momentum distribution, and show the momenta through parametric resonance with the oscillations of the population imbalance observed at small times. We show that through this resonance it of 1D coupled gases we find similar behavior for short times, but quantum fluctuations destroy the self trapped state by production of particle pairs of opposite is caused by singular \( \pm \pi n \) scattering processes and can be understood by analogy to the Kondo effect, both at strong and weak coupling, with the possibility scattering processes and can be understood by analogy to the Kondo effect, both at strong and weak coupling, with the possibility of a quantum phase transition where \( \Omega(\pm\pi n) \) jumps to zero with increasing coupling. The low energy singularities in the impurity spectral function can be understood on the same footing.

This work is in part supported by the office of the Dean of Science, UBC, NSERC (Canada), Canadian Institute for Advanced Research, and the A. P. Sloan foundation.

2:42PM L16.00002 Vortex lattice locking in rotating two-component Bose-Einstein Condensates, RYAN BARNETT, EDWARD CHEN, Caltech, MASON PORTER, Oxford, HANS PETER BUCHLER, Stuttgart, GIL REFAEL, Caltech — The vortex density of a rotating superfluid, divided by its particle mass, dictates a superfluid’s angular velocity through the Feynman relation. To find how the Feynman relation applies to superfluid mixtures, we investigate a rotating two-component Bose-Einstein condensate, composed of bosons with different masses. We find that in the case of sufficiently strong interspecies attraction, the vortex lattices of the two condensates lock and rotate at the drive frequency, while the superfluids themselves rotate at two different velocities, whose ratio is that of the particle masses of the two species. In this talk, I will characterize the vortex-locked state, establish its regime of stability, and find that it survives within a disk smaller than a critical radius, beyond which vortices become unbound. Finally, numerical solution of the coupled Gross-Pitaevskii equations in support of this will be presented.

2:54PM L16.00003 Quantum fluctuations of a Bose-Josephson junction on a quasi-one-dimensional ring trap, NICOLAS DIDIER, ANNA MINGUZZI, Université Joseph Fourier, Laboratoire de Physique et de Modélisation des Milieux Condensés, C.N.R.S., ROBERTA CITRO, Università degli Studi di Salerno, Dipartimento di Fisica “E. R. Caianiello”, 84081 Baronissi (Sa), Italy, FRANK W.J. HEKKING, Université Joseph Fourier, Laboratoire de Physique et de Modélisation des Milieux Condensés, C.N.R.S. — Ring traps for ultracold atomic gases are becoming experimentally feasible. We study the theory of quantum fluctuations of a Bose-Einstein condensate confined to a quasi-one-dimensional ring trap where a Josephson junction is realized with a localized barrier potential. We consider the situation where the transverse confinement of the trap is so tight that only longitudinal quasi-1D motion is allowed along the ring. The condensate is treated as a Luttinger liquid and the low energy properties are described within the bosonization formalism. For a very large barrier, we study the one-particle density-matrix including the correction due to the density fluctuations. Our analysis reveals different power law decays depending on the location of the probed points, i.e. whether they are chosen in the bulk or at the edge of the ring under consideration. This quasi-long range order could be probed using an interference measurement. In the Tonks-Girardeau limit, the density-density correlation function tends to the exact result obtained from the Bose-Fermi mapping. The momentum distribution is calculated and compared to the result for a very small barrier. Furthermore, for a barrier of finite height, within the renormalization group approach, we study how quantum fluctuations reduce the effective Josephson coupling strength.

3:06PM L16.00004 Detecting statistics of quasiparticles using dynamical probes, CLAUDIA DE GRANDI, ROMAN BARANKOV, ANATOLI POLKOVNIKOV, Boston University — We study a time-dependent sine-Gordon model in the range of the coupling constant (Luttinger parameter) where the quasiparticles excitations change from massive bosons to free fermions. We find that, if we include the effects of finite temperature, the non-adiabatic response to slow perturbations is enhanced for the bosonic case and reduced for the fermionic one with respect to zero temperature. The signature of this bunching (anti-bunching) behaviour can also be seen at zero temperature by analyzing the second order corrections of a perturbative approach in the number of quasiparticles created. This suggests the existence of a crossover (for the Luttinger parameter) that separates systems with Bose-like statistics from systems with fermi-like statistics, and therefore time-dependent perturbations to the system can be used to probe the statistics of the quasiparticles. We show how this model is relevant for cold atoms experiments that realize splitting and merging of two one-dimensional Bose gases.

3:18PM L16.00005 Motion of an impurity in a one-dimensional quantum liquid, AUSTEN LAMACRAFT, University of Virginia — We consider the motion of an impurity particle in a general one-dimensional quantum fluid at zero temperature. The dispersion relation \( \Omega(P) \) of the impurity is strongly affected by interactions with the fluid as the momentum approaches \( \pm \pi n \hbar, \pm 3\pi n \hbar, \ldots \), where \( n \) is the density. This behavior is caused by singular \( \pm 2\pi n \hbar \) scattering processes and can be understood by analogy to the Kondo effect, both at strong and weak coupling, with the possibility of a quantum phase transition where \( \Omega(\pm\pi n) \) jumps to zero with increasing coupling. The low energy singularities in the impurity spectral function can be understood on the same footing.

3:30PM L16.00006 Breakdown of Macroscopic Quantum Self Trapping in Coupled 1D Bose Gases, RAFAEL HIPOLITO, ROMAN BARANKOV, ANATOLI POLKOVNIKOV, Boston University — Two coupled 1D Bose-Einstein condensates with a large population imbalance exhibit macroscopic quantum self-trapping if the ratio of interaction energy to the coupling energy between the two gases is above a critical value. Above the self trapping transition, one sees only small amplitude high frequency oscillations of the population difference. In the analogous case of 1D coupled gases we find similar behavior for short times, but quantum fluctuations destroy the self trapped state by production of particle pairs of opposite momenta through parametric resonance with the oscillations of the population imbalance observed at small times. We show that through this resonance it is possible, by choosing the parameters of the system appropriately, to produce an interacting 1D Bose gas with sharp momentum distribution, and show the conditions that the system must satisfy in order to produce such a state.
3:42PM L16.00007 The Mass of a Spin Vortex, in a Bose Einstein Condensate. ARI TURNER, University of California Berkeley — Ferromagnetic condensates can have both spin-current and charge-current vortices. A moving charge-vortex experiences the Magnus force, perpendicular to its motion, when it moves. This effective “magnetic field” is so strong that it dominates the inertial term in Newton’s law; therefore it is not possible to set a charge-vortex moving at an arbitrary speed relative to the condensate. As we will show, a spin-vortex can move “inertially” through a condensate and resists acceleration with a mass.

3:54PM L16.00008 Unusual states of vortex matter in interacting multicomponent Bose-Einstein condensates, EGOR BABAEEV, University of Massachusetts Amherst, ESKIL DAHL, ASLE SUDBO, NTNU Trondheim — A striking property of a single-component superfluid under rotation, is that a broken symmetry in the order parameter results in a broken translational symmetry, a vortex lattice. If translational symmetry is restored by means of rotation disorder, as for example in a laser driven superfluid, then the broken translational symmetry is restored. We show that for interacting mixtures of Bose-condensate (with a dissipationless intercomponent drag), new situations arise. A phase disordered nonsuperfluid component can break translational symmetry in response to rotation due to interaction with a superfluid component. In a different regime instead of a vortex lattice, the system forms a highly disordered vorticity which completely undergoes merger and reconnecting processes involving different types of vortices, with a breakdown of translational symmetry only in a statistical sense.

4:06PM L16.00009 Normal modes of a ring-shaped BEC with vortices, SUNGJONG WOO, Univ of Mass Lowell, YOUNG-KYUN KWON, Kyung Hee University, Univ of Mass Lowell — Recently, a ring-shaped BEC was realized experimentally at NIST and long lasting perpetual current was observed. Using Bogoliubov-de Gennes equations, we have analyzed dynamics of such a non-simply connected rotating condensate system with quantized vortices. Surface modes of a simply connected rotating BEC are known to be associated with driven vortices that can make interactions with the vortex lattice that exists due to the rotation. In our current work, it has been found that stable vortex dipoles or velocity dipoles that do not exist in a normal mode for a simply connected BEC, exist in a non-simply connected case generating “inner” surface modes. The interactions of such inner surface modes with quantized changes as well as the stability of the perpetual current related to the low lying excitations will be discussed. How the angular dispersion relation changes as a BEC makes a transition from a simply connected to a ring-shaped one will also be presented.

4:18PM L16.00010 Hierarchies of Supercurrents in Multicomponent Atomic Josephson Vortices, VITALIY KAUROV, CSI, CUNY — We show that a quasi-1D long atomic Josephson junction [1,2] containing a mixture of BECs can sustain multi-component Josephson vortices (mJV). A new exact soliton solution is given to describe a stationary mJV in the general N-component case. Depending on system parameters (scattering lengths, tunneling strengths, and chemical potentials) Josephson supercurrents of different components form a hierarchy according to their intensity and proximity to phase slip. By tuning the parameters it is possible to turn off or on particular currents using the JV – dark soliton interconversion effect [1,2]. Inside the mJV different components may circulate either in the same or opposite directions resulting in bulk super-counter-flow in the latter case. The weak tunneling limit can be described by a modified Sine-Gordon model. An approximate solution for mJV propagating along the junction is found for the two-component case. The degeneracy of stationary mJV with respect to co-flow or counter-flow configurations is lifted by the uniform motion of mJV. Which configuration is energetically preferable depends on the interspecies scattering length. [1] V. M. Kaurow and A. B. Kuklov, Phys. Rev. A 71, 016101-R (2005). [2] V. M. Kaurow and A. B. Kuklov, Phys. Rev. A 73, 013632 (2006).

4:30PM L16.00011 Rotating Bose-Einstein condensates at the phase transition point, MAHIR HUSSEIN, Max Planck Institut fur Physik Komplexer Systeme, Dresden, Germany, PIET VAN ISACKER, Grand Accelerateur National d’Ions Lourds, KLAUS BARTSCHAT, Drake University, OLEG VOROV, University of North Carolina, Charlotte — Here we give analytic description of the phase transitions in the rotating Bose-Einstein condensate of weakly interacting atoms in a magnetic trap [1,2]. The analytic solution allows one to classify the instabilities in the condensates which occur when the rotational speed is increased [3]. In the case of predominantly repulsive interactions, the transition corresponds to the vortex entry the condensate. The transition to the Abrikosov state has follows if the rotational speed is increased further. In the case of predominantly attractive interactions, the transition corresponds to the escape of the condensate from the trap at the critical speed. [1] O. K. Vorov, P. Van Isacker, M. S. Hussein and K. Bartschat, Phys. Rev. Lett. 95, 230406 (2005). [2] O. K. Vorov, M. S. Hussein and P. Van Isacker, Phys. Rev. Lett. 90, 200402 (2003). [3] O. K. Vorov, P. Van Isacker, M. S. Hussein and K. Bartschat, to be submitted to Nature (2007). Supported by NSF (USA), CEA (France).

4:42PM L16.00012 Strongly Interacting Quantum gases using spin-Coherent state Representation, RADHA BALAKRISHNAN, Institute of Mathematical Sciences, Chennai, India, INDUBALA SATIJA, George Mason University, Fairfax, VA — For strongly interacting boson gas, spin-coherent states representation may provide a useful description of the Bose-Einstein Condensate as it encodes fluctuations and depletion. We investigate the the non-linear evolution equation for the order parameter obtained using spin-coherent states. The equation is not of the GPE-type and exhibits local fluctuations and in the limit of small order parameter, it reduces to the GPE equation. We compare and contrast the quasi-particle excitation and the vortex excitations of this system with that of weakly interacting quantum gases described by GPE equation. For a variety of problems, implication of this description of quantum gases will be discussed.

4:54PM L16.00013 Dynamics of spinor condensates near point-group symmetric ground states, GIL REFAEL, RYAN BARNETT, Caltech. DANIEL PODOLSKY, University of Toronto — The mean-field ground state of spin- S BEC’s often exhibits a high degree of symmetry, which only becomes apparent when considering the 25 reciprocal spin-states: coherent spin-states orthogonal to the ground state. Our presentation will concentrate on a description of the dynamics of spinor-condensates using these reciprocal states. First, we will present the resulting hydrodynamic Euler equations, which generalize Mermi-Nico relations to higher spin. Second, we will use the reciprocal states and their hidden point-group symmetry to construct the Goldstone and optical spin-wave modes of the spinor condensates. Finally, we will present a mapping between the spin-wave modes, and the wave functions of electrons in atoms, where the spherical symmetry is degraded by a crystal field.

Tuesday, March 17, 2009 2:30PM - 5:30PM —
Session L17 GQI: Superconducting Flux Qubits and Qubit Amplifiers and Readouts 318

2:30PM L17.00001 Behavior of a Josephson Flux Qubit on a Sapphire Substrate, ANTHONY PRZYBYSZ, E. CROWE, H. KNOW, B.K. COOPER, R.M. LEWIS, University of Maryland, JQI, CNAM, B.S. PALMER, The Laboratory for Physical Science, JQI, J.R. ANDERSON, C.J. LOBB, F.C. WELLSTOOD, University of Maryland, JQI, CNAM — We discuss the design, fabrication, and testing of a Nakamura-style [1] flux qubit. The device consists of a four-Josephson junction qubit loop that is directly coupled to a small dc SQUID, which is used for detection. The device was built on a sapphire substrate using electron beam lithography and double angle evaporation to form the Al/Alo/Al tunnel junctions. A 200 nm thick layer of aluminum was deposited on the e-beam resist in order to prevent charge effects during the lithography. Three of the junctions in the qubit loop were 100 nm x 250 nm, and the fourth was 100 nm x 150 nm. The large junctions are the main contribution to the inductance of the qubit loop, and the smaller junction creates an energy splitting of 1-10 GHz between the two circulating current states. The SQUID junctions were 100 nm x 2000 nm, and the critical current of the detection SQUID was 240 nA. We present the results of ongoing measurements on the behavior of the device at 25 mK. This project was funded by the JQI, LPS, and CNAM. [1] F. Yoshihara, Y. Nakamura, et al., “Decoherence of Flux Qubit Due to 1/F Flux Noise,” PRL 97, 167001 (2006).

2:42PM L17.00002 Josephson Vortices in a Strongly Interacting Bose-Einstein Condensate, DMITRII GORELKO, Srinivas KOTILRA, University of Maryland, JQI, CNAM — We discuss the design, fabrication, and testing of a Josephson vortex qubit. The device consists of a Josephson vortex loop that is coupled to a small dc SQUID, which is used for detection. The device was built on a sapphire substrate using electron beam lithography and double angle evaporation to form the Al/Alo/Al tunnel junctions. A 200 nm thick layer of aluminum was deposited on the e-beam resist in order to prevent charge effects during the lithography. Three of the junctions in the qubit loop were 100 nm x 250 nm, and the fourth was 100 nm x 150 nm. The large junctions are the main contribution to the inductance of the qubit loop, and the smaller junction creates an energy splitting of 1-10 GHz between the two circulating current states. The SQUID junctions were 100 nm x 2000 nm, and the critical current of the detection SQUID was 240 nA. We present the results of ongoing measurements on the behavior of the device at 25 mK. This project was funded by the JQI, LPS, and CNAM. [1] F. Yoshihara, Y. Nakamura, et al., “Decoherence of Flux Qubit Due to 1/F Flux Noise,” PRL 97, 167001 (2006).
2:42PM L17.00002 IBM’s experimental quantum computing effort. MATTHIAS STEFFEN, IBM, DAVID DIVINCENZO, MATTHEW FARINELLI, GEORGE KEEFE, MARK KETCHEN, SHWETANK KUMAR, FRANK MILLIKEN, MARY BETH ROTHWELL, JIM ROZEN — We present our experimental quantum computing effort and discuss results on flux and phase qubits.

2:54PM L17.00003 Tuning the gap of the superconducting flux qubit. ARKADY FEDOROV, FLOOR PAAUW, KEES HARMANS, HANS MOOIJ, Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600 GA Delft, The Netherlands — Recent advances in experiments with the flux qubits include demonstration of single and two qubit quantum gates as well as a coupling between the flux qubit and a harmonic oscillator. It was also experimentally confirmed that the best coherence properties were achieved when the qubit was kept at the symmetry point. For these conditions the qubit’s energy level splitting is minimal (the gap) and determined solely by the quantum tunnelling in the double-well potential. However, since the potential barrier and the gap of the conventional flux qubit are fully fixed by the fabrication, one needs to tune the qubits out of the symmetry point in order to bring it in resonance with another quantum system. We overcome this limitation by introducing the change in the qubit design and demonstrated the tuning of the gap over a range of several Gigahertz within a few nanoseconds. We believe this could be an important step toward the coupling of the flux qubit to another qubit or the quantum bus. This control also allows a more extensive study of the relaxation time of the qubit as a function of the gap size within a constant environment.

3:06PM L17.00004 Ultra-strong coupling regime of cavity QED with flux qubits. JEROME BOURASSA, ALEXANDRE BLAIS, Universite de Sherbrooke — With improved dephasing rate and coupling strength, the transmon qubit has recently been used to reach the strong coupling regime of cavity QED [1,2]. With the transmon however, these improvements are done at the expense of lower anharmonicity compared to the Cooper-pair box. Here we present an alternative approach where a flux qubit is coupled to the transmission line. As was recently shown experimentally [1], very strong coupling can be obtained by directly connecting the qubit loop to the center conductor of the resonator whose local inductance is tuned to maximize the coupling. We will discuss how this system can be used to study the breakdown of the rotating-wave approximation and how the Λ-configuration of the energy levels of the flux qubit can be exploited.


3:18PM L17.00005 Amplitude spectroscopy of a superconducting artificial atom. WILLIAM OLIVER, MIT Lincoln Laboratory, DAVID BURNS, MIT, SERGIO VALENZUELA, CIN2-ICN Barcelona, MARK RUDNER, Harvard; LEONID LEVITO, TERRY ORLANDO, MIT — We introduce and demonstrate amplitude spectroscopy in a superconducting artificial atom [1]. A harmonic field at a fixed frequency drives the artificial atom through its energy-level avoided crossings. Spectroscopic information is obtained from the amplitude dependence of the system response. The resulting ‘spectroscopy diamonds,’ regions of parameter space in which state transitions occur, exhibit quantum interference patterns and population inversion which serve as a fingerprint of the atom’s energy spectrum. Using this approach, we determined the energy spectrum of a manifold of states with energies from hω 0.01 GHz to hω 120 GHz for a fixed driving frequency near only 0.16 GHz. The amplitude spectroscopy technique is complementary to frequency spectroscopy, providing a means to access, manipulate, and characterize quantum systems over broad bandwidths while using only a single drive frequency that may be orders of magnitude smaller than the energy scales being probed. [1] Berns et al., Nature 455, 51 (2008)

3:30PM L17.00006 Phase tomography of a strongly driven superconducting artificial atom. MARK RUDNER, Harvard University, ANDREI SHYTOV, University of Utah, LEONID LEVITO, DAVID BURNS, MIT, WILLIAM OLIVER, MIT Lincoln laboratory, TERRY ORLANDO, SERGIO VALENZUELA, MIT — In a recent experiment [1], amplitude spectroscopy of a superconducting qubit was demonstrated by driving the system with a strong rf field through a manifold of states spacing energies up to 120 GHz. The interference between repeated Landau-Zener transitions in a qubit swept through an avoided level crossing results in Stueckelberg oscillations in qubit magnetization. The resulting oscillatory patterns are a hallmark of the coherent strongly-driven regime in qubits, quantum dots and other two-level systems. The two-dimensional Fourier transforms of these patterns are found to exhibit a family of one-dimensional curves in Fourier space [2], in agreement with experiment [1]. We interpret these images in terms of the time evolution of the quantum phase of the qubit state and show that they can be used to probe dephasing mechanisms in the qubit. [1] D. M. Berns et al., Nature 455, 51 (2008). [2] M. S. Rudner et al., Phys. Rev. Lett. 101, 190502 (2008)

3:42PM L17.00007 Simultaneous cooling of an artificial atom and its neighboring quantum system. JIANQIANG YOU, Fudan University & RIKEN, YU-XI LIU, RIKEN, FRANCO NORI, University of Michigan & RIKEN — We propose an approach for cooling both an artificial atom (e.g., a flux qubit) and its neighboring quantum system, the latter modeled by either a quantum two-level system or a quantum resonator. The flux qubit is cooled by manipulating its states, following an inverse process of state population inversion, and then the qubit is switched on to resonantly interact with the neighboring quantum system. By repeating these steps, the two subsystems can be simultaneously cooled. Our results show that this cooling is robust and effective, irrespective of the chosen quantum systems connected to the qubit.

3:54PM L17.00008 Chirped nonlinear cavity for digital quantum state readout without switching. OFER NAAMAN, QNL, UC Berkeley, JOSÉ AUMENTADO, NIST, Boulder, LAZAR FRIEDLAND, Racah Institute of Physics, Hebrew University, Jerusalem, Israel, JONATHAN WURTELE, Department of Physics, University of California, Berkeley, IRFAN SIDDIQI, QNL, UC Berkeley — We observe a new phase-locking effect in a high-Q cavity embedding a Josephson junction driven with a chirped microwave signal. Above a critical drive amplitude, the cavity phase-locks to the drive and its oscillation amplitude grows with time. Below threshold, the cavity dephases from the drive and its amplitude remains small. The transition to phase-locking is associated with a sharp threshold sensitive to the junction IO, and can be used for digital detection of quantum states. This detector smoothly evolves into one oscillation state or the other without relying on any switching process.

4:06PM L17.00009 Lumped-element microwave resonant circuit with a dc SQUID. M.P. DEFEO, C. SONC, T.W. HEITMANN, K. YU, B.L.T. PLOURDE, Syracuse University, R. MCDERMOTT, University of Wisconsin — We have fabricated lumped-element microwave resonant circuits consisting of a dc SQUID shunted with a capacitor formed from superconducting layers. Adjusting the SQUID bias conditions changes its Josephson inductance, thus varying the resonant frequency. We discuss the possibility of time-domain monitoring of the oscillations in these circuits and their potential use in a new readout scheme for superconducting qubits.

4:18PM L17.00010 Qubit decoherence due to a Josephson bifurcation amplifier trapped in one of... FRANK WILHELM, IOANA SERBAN, University of Waterloo, MARK DYKMAN, Michigan State University — We investigate the relaxation of a superconducting flux qubit for the case when its detector, the Josephson bifurcation amplifier, remains latched in one of its two (meta)stable states. We observe a qualitatively different behavior for the two different attractors, and interpret the result as the combined effect of the amplitude of the detector’s response to external driving and the effective curvature of the detector’s basins of attraction in a rotating frame, in the proximity of the stable points. We address the question of the proper version of detailed balance for the qubit.

1Work supported in parts by NSERC and NSF
4:30PM L17.00011 Parametric Resonators for Quantum Information Applications, C.M. WILSON, M. SANDBERG, F. PERRSON, I. HOI, G. JOHANSSON, V. SHUMEIKO, P. DELSING, Chalmers University, T. DUTY, U. Queensland — We have fabricated and characterized tunable superconducting transmission line resonators. To change the resonance frequency, we modify the boundary condition at one end of the resonator through the tunable Josephson inductance of a SQUID. We demonstrate a large tuning range, high quality factors and that we can change the frequency of a few-photon field on a time scale orders of magnitude faster than the photon lifetime. When parametrically pumped at twice their resonance frequency, the devices can act as parametric amplifiers. When pumped strongly, a threshold is crossed where the resonators oscillate spontaneously. Within this regime of parametric oscillations, the devices can exist in a variety of dynamical states. We observe a rich pattern in the dynamics of switching between these states. We study the possibility of using this dynamical bifurcation for qubit readout. Finally, recent theoretical work has suggested that it may be easier to observe dynamical tunneling in this system than in the Duffing oscillator.

4:42PM L17.00012 The effects of higher-harmonic mode coupling in quarter-wave SQUID parametric amplifiers, MINHYEA LEE, LAFE SPIETZ, JOSE AUMENTADO, National Institute of Standards and Technology — Recent interest in quarter-wave SQUID-based parametric amplifiers has motivated concerns regarding the coupling of higher harmonic modes to the operating frequency mode. We will present experiments in which the harmonic mode coupling is attempted to measure. We will also discuss the effect of higher mode coupling on noise performance and gain, focusing on whether this mode coupling limits practical amplifier performance.

4:54PM L17.00013 Nonlinear dissipative filters for measurement protection on superconducting qubits1, POL FORN-DIAZ, RAYMOND SCHOUTEN, KEES HARMANS, HANS MOOIJ, TU Delft. Kavli Institute of Nanoscience — Measurements on superconducting qubits require the system to be well isolated from noise sources if its quantum state is not being accessed. This ensures that decoherence induced by the measurement apparatus is minimized. The need to have slow (sub-GHz) and fast (GHz) lines to measure and control the state of the qubit is difficult to combine with the requirement to attenuate the noise over a broad spectral range. To overcome this problem, we have built a new type of non-linear coaxial copper powder filter with a Josephson junction in its inside. The junction in the filter acts as a shorting switch. For low frequencies, the junction acts as a shortcut to ground, and high frequencies are absorbed in the metallic powder. The Josephson junction critical current is taken such that when sending a pulse to probe the measurement device (a DC SQUID in our case), the junction in the filter switches to the voltage state, thus reaching the SQUID to perform the measurement. A minimum noise suppression of 40 dB is obtained, while allowing ns pulses to be transported.

5:06PM L17.00014 Development of a Microwave Resonator for Qubit Read-out1, ZAEILL KIM, V. ZARETSKEY, Department of Physics, University of Maryland, K. D. OSBORN, Laboratory for Physical Sciences, F. C. WELSTOOD, IQI, CNAM, Department of Physics, University of Maryland, B. S. PALMER, Laboratory for Physical Sciences — We have designed and fabricated a “lumped-element” thin-film superconducting Al microwave resonator on sapphire to be used to read out a Cooper-pair box. The resonator consists of a meandering inductor and an interdigitated capacitor coupled to a transmission line. At T=30 mK and on resonance at 5.578 GHz, the transmission through the transmission line decreases by 15 dB and the loaded quality factor is 60,000. We have studied the temperature dependence of our resonator at temperatures as high as 500 mK and compared it to the Mattis-Bardeen theory. Coupling of this resonator to a Cooper-pair box qubit will be discussed.

5:18PM L17.00015 Resolving Vacuum Fluctuations in an Electrical Circuit by Measuring the Lamb Shift, ANDREAS FRAGNER, MARTIN GOPPL, ETH Zurich, ALEXANDRE BLAIS, Universite de Sherbrooke, ANDREAS WALLRAFF, ETH Zurich, ETH QUANTUM DEVICE TEAM — Quantum theory predicts that empty space is not truly empty. Even in the absence of any particles or radiation, in pure vacuum, virtual particles are constantly created and annihilated. In an electromagnetic field, the presence of virtual photons manifests itself as a small renormalization of the energy of a quantum system, known as the Lamb shift. We present an experimental observation of the Lamb shift in a solid-state system. The strong dispersive coupling of a superconducting electronic circuit acting as a quantum bit (qubit) to the vacuum field in a transmission-line resonator leads to measurable Lamb shifts of up to 1.4% of the qubit transition frequency. The qubit is also observed to couple more strongly to the vacuum field than to a single photon inside the cavity, an effect that is explained by taking into account the limited anharmonicity of the higher excited qubit states.

5:30PM L18.00001 Recent Advances in X-Ray Free Electron Lasers1, KWANG-JE KIM, Argonne National Laboratory — X-ray free electron lasers(FELs) are undergoing an exciting development. They will soon become a reality with the commissioning of the LCLS in early next year, soon followed by Spring 8 X-FEL and the European XFEL at Hamburg. Intense, coherent pulses of x-rays from these machines will permit exploration of the atomic world with spatial and temporal precisions hitherto not feasible. After these first generation x-ray FELs based on self-amplified spontaneous emission (SASE) in a single pass high-gain system, the next generation devices for higher performance and/or smaller and lower cost are under various stages of development. In the soft x-ray region, seeded FELs with high harmonic generated (HHG) laser input will produce coherent output in a shorter wavelength region. The x-ray FEL oscillator (XFELO) provides ultra-narrow spectral resolution. The XFELO employs optical cavity formed by Bragg reflectors, delivering temporally and spatially coherent hard x-rays, with meV spectral resolution. Its peak spectral brightness is similar to but the average spectral brightness is about five orders of magnitudes higher than LCLS.

5:42PM L17.00016 The effects of higher-harmonic mode coupling in quarter-wave SQUID parametric amplifiers, MINHYEA LEE, LAFE SPIETZ, JOSE AUMENTADO, National Institute of Standards and Technology — Recent interest in quarter-wave SQUID-based parametric amplifiers has motivated concerns regarding the coupling of higher harmonic modes to the operating frequency mode. We will present experiments in which the harmonic mode coupling is attempted to measure. We will also discuss the effect of higher mode coupling on noise performance and gain, focusing on whether this mode coupling limits practical amplifier performance.

5:54PM L17.00017 Nonlinear dissipative filters for measurement protection on superconducting qubits1, POL FORN-DIAZ, RAYMOND SCHOUTEN, KEES HARMANS, HANS MOOIJ, TU Delft. Kavli Institute of Nanoscience — Measurements on superconducting qubits require the system to be well isolated from noise sources if its quantum state is not being accessed. This ensures that decoherence induced by the measurement apparatus is minimized. The need to have slow (sub-GHz) and fast (GHz) lines to measure and control the state of the qubit is difficult to combine with the requirement to attenuate the noise over a broad spectral range. To overcome this problem, we have built a new type of non-linear coaxial copper powder filter with a Josephson junction in its inside. The junction in the filter acts as a shorting switch. For low frequencies, the junction acts as a shortcut to ground, and high frequencies are absorbed in the metallic powder. The Josephson junction critical current is taken such that when sending a pulse to probe the measurement device (a DC SQUID in our case), the junction in the filter switches to the voltage state, thus reaching the SQUID to perform the measurement. A minimum noise suppression of 40 dB is obtained, while allowing ns pulses to be transported.

6:06PM L17.00018 Development of a Microwave Resonator for Qubit Read-out1, ZAEILL KIM, V. ZARETSKEY, Department of Physics, University of Maryland, K. D. OSBORN, Laboratory for Physical Sciences, F. C. WELSTOOD, IQI, CNAM, Department of Physics, University of Maryland, B. S. PALMER, Laboratory for Physical Sciences — We have designed and fabricated a “lumped-element” thin-film superconducting Al microwave resonator on sapphire to be used to read out a Cooper-pair box. The resonator consists of a meandering inductor and an interdigitated capacitor coupled to a transmission line. At T=30 mK and on resonance at 5.578 GHz, the transmission through the transmission line decreases by 15 dB and the loaded quality factor is 60,000. We have studied the temperature dependence of our resonator at temperatures as high as 500 mK and compared it to the Mattis-Bardeen theory. Coupling of this resonator to a Cooper-pair box qubit will be discussed.

6:18PM L17.00019 Resolving Vacuum Fluctuations in an Electrical Circuit by Measuring the Lamb Shift, ANDREAS FRAGNER, MARTIN GOPPL, ETH Zurich, ALEXANDRE BLAIS, Universite de Sherbrooke, ANDREAS WALLRAFF, ETH Zurich, ETH QUANTUM DEVICE TEAM — Quantum theory predicts that empty space is not truly empty. Even in the absence of any particles or radiation, in pure vacuum, virtual particles are constantly created and annihilated. In an electromagnetic field, the presence of virtual photons manifests itself as a small renormalization of the energy of a quantum system, known as the Lamb shift. We present an experimental observation of the Lamb shift in a solid-state system. The strong dispersive coupling of a superconducting electronic circuit acting as a quantum bit (qubit) to the vacuum field in a transmission-line resonator leads to measurable Lamb shifts of up to 1.4% of the qubit transition frequency. The qubit is also observed to couple more strongly to the vacuum field than to a single photon inside the cavity, an effect that is explained by taking into account the limited anharmonicity of the higher excited qubit states.

Tuesday, March 17, 2009 2:30PM - 5:30PM – Session L18 DPB: Advanced Techniques in Acceleration and Coherent Radiation 319

2:30PM L18.00001 Recent Advances in X-Ray Free Electron Lasers1, KWANG-JE KIM, Argonne National Laboratory — X-ray free electron lasers(FELs) are undergoing an exciting development. They will soon become a reality with the commissioning of the LCLS in early next year, soon followed by Spring 8 X-FEL and the European XFEL at Hamburg. Intense, coherent pulses of x-rays from these machines will permit exploration of the atomic world with spatial and temporal precisions hitherto not feasible. After these first generation x-ray FELs based on self-amplified spontaneous emission (SASE) in a single pass high-gain system, the next generation devices for higher performance and/or smaller and lower cost are under various stages of development. In the soft x-ray region, seeded FELs with high harmonic generated (HHG) laser input will produce coherent output in a shorter system. Drastic improvement in hard x-ray region is possible with new types of electron injectors producing electron beams with an order of magnitude smaller emittance. Hard x-ray FELs can be built with an order of magnitude smaller electron energy and thus with a significant savings in the cost. The Spring-8 FEL is a first step in this direction. Novel types of FELs are possible; ultra-short SASE providing sub-fs time-resolution and x-ray FEL oscillator (XFELO) providing ultra-narrow spectral resolution. The XFELO employs optical cavity formed by Bragg reflectors, delivering temporally and spatially coherent hard x-rays, with meV spectral resolution. Its peak spectral brightness is similar to but the average spectral brightness is about five orders of magnitudes higher than LCLS.

3:06PM L18.00002 Novel Techniques for the Generation of Ultrashort Attosecond Pulses of Coherent Radiation1, ALEXANDER ZHOLENTS, Lawrence Berkeley National Laboratory — Revealing the laws of Nature often require developing unique experimental tools. In this talk I will discuss new tools that will enable probing of matter with attosecond time resolution and Angstrom spatial resolution. Their emergence is largely due to the spectacular progress in development of x-ray free electron lasers and similar progress in generation of the ultra-short light pulses in optics.
3:42PM L18.00003 Photonic Band-gap Materials for Particle Acceleration, GENNADY SHVETS, UT Austin — No abstract available.

4:18PM L18.00004 Emerging Long-Wavelength Coherent Light Sources—from the infrared to soft X-rays¹, JOSEPH BISOGNANO, SRC-University of Wisconsin — The theory and techniques of accelerator-based coherent light sources will be discussed. Application of these ideas to the design of user facilities from the IR to soft X-rays will be presented, including world-wide initiatives for next generation light source R&D and construction at these longer wavelengths.


Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L19 DMP DPOLY: Focus Session: Ionically Gated and Conventional OFETs and Related Devices 320

2:30PM L19.00001 All-Printed Low Voltage Operation Polymer Transistors and Circuits Based on Ion Gel Gate Dielectrics, YU XIA, JEONG HO CHO, MINGJING HA, Department of Chemical Engineering and Materials Science, University of Minnesota, MICHAEL REENN, Optomec, Inc, C. FRISBIE, Department of Chemical Engineering and Materials Science, University of Minnesota, OPTOMEC, INC COLLABORATION — A key challenge in the development of organic electronics lies in the realization of high quality devices with low cost. In this presentation, we demonstrate high performance polymer transistors and circuits with all components fabricated by a commercial aerosol jet printing technique. Printing saves the device manufacturing cost through its simple procedure, fast speed, high throughput and low waste of materials. Furthermore, by employing a specially designed ion gel as the gate dielectric material, ultra-high density carrier accumulation (> 10¹⁴ cm⁻²) can be achieved in the transistor channel, which results in an exceptionally large transconductance of 10 µS/µm. Our typical transistors have mobility higher than 1cm²/Vs and frequency response up to 10 kHz. Inverters, NAND and NOR logic circuits and ring oscillators have been realized as well, with low operation voltage, fast speed and high gain. In addition, the high polarizability of the gate dielectric allows us to print the gate electrode of each single transistor along with its source and drain electrodes at the same time in a coplanar architecture, which significantly simplifies the fabrication procedure.

2:42PM L19.00002 Non-volatile Ferroelectric Poly(vinylidene fluoride-co-trifluoroethylene) Memory based on Single Crystalline Triisopropylisilyl ethynyl Pentacene Field Effect Transistor², SEOK JU KANG, INSUNG BAE, YOUN JUNG PARK, TAE HO PARK, JINWOO SUNG, CHEOLMIN PARK, Yonsei university — We develop a new type of non-volatile ferroelectric poly(vinylidene fluoride-co-trifluoroethylene) (P(VDF-TrFE)) memory based on Organic Thin Film Transistor (OTFT) with single crystal Triisopropylisilyl ethynyl pentacene (TIPS-PEN) active layer. A bottom gate OTFT was fabricated with thin P(VDF-TrFE) film gate insulator on which 1D ribbon type single crystal TIPS-PEN grown via solvent exchange method was positioned between Au source and drain electrode. As consequences a memory device exhibits substantially stable source-drain current modulation with the hysteresis ON/OFF ratio larger than 10³, superior to a ferroelectric P(VDF-TrFE) OTFT with vacuum evaporated pentacene layer. Data retention longer than 5x10⁶ seconds was achieved in ambient condition by incorporating an interlayer between gate electrode and P(VDF-TrFE) thin film. The device is environmentally stable for more than 40 days without additional passivation.

2:54PM L19.00003 Polymer Electrolyte Gated Inorganic Transistors, ANOOP SINGH DHOOIT, Cavendish Laboratory, University of Cambridge, CASEY ISRAEL, XAVIER MOYA, STUART WIMBUSH, Department of Materials Science and Metallurgy, University of Cambridge, TIM BENSEMAN, Cavendish Laboratory, University of Cambridge, JUDITH MACMANUS-DRISCOLL, Department of Materials Science and Metallurgy, University of Cambridge, JOHN COOPER, Cavendish Laboratory, University of Cambridge, NEIL MATHUR, Department of Materials Science and Metallurgy, University of Cambridge, RICHARD FRIEND, Cavendish Laboratory, University of Cambridge — Electric field-induced charge at the interface between gate dielectric and semiconductor is the basis of current semiconductor technology. We report that it is possible to use polymer electrolyte gate inorganic materials, and to achieve field-induced ‘doping’ equivalent to a full surface coverage of charged ions per unit cell area. Very high field-induced carrier densities, ~10¹⁵ cm⁻², in the transistor channel of La₉0₅Ca₁₅₀₇₋ₓMnO₃ devices enable modulation of the Curie temperature of over 30 K. We have also used electrolyte gating of the superconductor YBa₂Cu₃O₇₋ₓ to modulate the onset of superconductivity. This creates an exciting opportunity for use of the electrolyte as gate dielectric in a wide variety of inorganic materials to explore formerly inaccessible band-filling regimes without the need for chemical substitution and additional disorder.

3:06PM L19.00004 Employing ‘Liquid Gap’ Transistors to Examine the Mobility-Carrier Density Relation in Polymer and Single Crystal Organic Semiconductors¹, DANIEL FRISBIE, University of Minnesota — It is generally known that the carrier mobility in organic semiconductors can depend on carrier density, but the precise relationship hinges on the degree of structural order and the dielectric polarizability at the organic/dielectric interface. We have fabricated both single crystal and polymer transistors using the PDMS stamp approach pioneered by Podzorov and Rogers [1], where we have replaced the usual ‘air gap’ in these structures with liquids having different dielectric constants. This structure allows us to examine transport in single crystals and polymer semiconductors as a function of tunable dielectric constant and also charge density. We find striking differences in transport behavior for organic single crystals versus polymer semiconductor films using these liquid dielectric transistors. For organic single crystals such as rubrene, the carrier mobility does not seem to be a function of charge density but does strongly depend on the liquid dielectric constant, in keeping with previous results reported by Morpurgo [2] on the effects of dielectric polarizability. For polymer semiconductors, the effect of charge density is overwhelming; there is a strong increase in charge mobility with increasing carrier concentration, following a power law. These results are already largely known, but the ‘liquid gap’ transistors provide a convenient testbed for examining these effects side-by-side for different materials in the same device. We will describe the device fabrication and the nature of our results, as well as discuss the origins of the very different behavior for single crystals versus polymer semiconductor films. 1) Sundar, V.C., et al. Science 303 (2004) 1643. 2) Hulea, I. N., et al. Nature Mater. 5 (2006) 982.

¹This work was supported by the NSF MRSEC Program.
properties of the semiconductor materials as well as their interfaces with contacts and substrates. These devices can be operated in aqueous environment as efficient ion-to-electron converters, thus providing an interface between the worlds of biology and electronics and also a unique platform for the study of organic/organic and organic/metal interfaces in liquids. Using photolithography, surface engineering and micro-fluidics we have developed several technique to fabricate OECTs having different geometries. This allows us to study the basic electronic properties and the sensing response of devices in order to understand their mechanism of operation. We studied how the dimensions of the transistors (in particular on the gate/channel area ratio) and the gate electrode material (metal or polymer) can be used to tune the device response for sensing of different species. The effect of the electrolyte on device response was evaluated studying transistors in aqueous electrolytes and ionic liquids. The detection limit of OECTs based sensors having different geometry, was analyzed for hydrogen peroxide, a species involved in glucose sensing.

3:42PM L19.00005 Organic electrochemical transistors for sensing applications. FABIO CICORA1,2, SANG YOON YANG, JOHNAH A. DEFRANCO, GEORGE G. MALLIARAS, MSE/Cornell University, ORGANIC ELECTRONICS LABORATORY CORNELL TEAM — The application of organic semiconductor devices to chemical and biological sensors seems to be a great fit. A promising approach towards organic-based sensors involves the use of organic electrochemical transistors (OECTs). These devices can be operated in aqueous environment as efficient ion-to-electron converters, thus providing an interface between the worlds of biology and electronics and also a unique platform for the study of organic/organic and organic/metal interfaces in liquids. Using photolithography, surface engineering and micro-fluidics we have developed several technique to fabricate OECTs having different geometries. This allows us to study the basic electronic properties and the sensing response of devices in order to understand their mechanism of operation. We studied how the dimensions of the transistors (in particular on the gate/channel area ratio) and the gate electrode material (metal or polymer) can be used to tune the device response for sensing of different species. The effect of the electrolyte on device response was evaluated studying transistors in aqueous electrolytes and ionic liquids. The detection limit of OECTs based sensors having different geometry, was analyzed for hydrogen peroxide, a species involved in glucose sensing.

1also at CNR/IFN Trento (Italy)

3:54PM L19.00006 Contact resistance and lifetime of organic thin film transistors. GVIDO BRATINA, ANDRÁZ PETROVIC, University of Nova Gorica — We have used ed electric charge transport measurements coupled to Kelvin force probe microscopy of pentacene organic thin film transistors (OTFT’s) to monitor the evolution of contact resistance as a function of time of exposure to ambient air. Or results demonstrate that exposure of OTFTs to ambient air for extended periods of time, results in two competitive mechanisms that are responsible for observed variation in drain-current. Initially, relatively fast oxygen doping through electronegativity-related creation of holes increases the carrier concentration and therefore increases the drain current. Slower, and persistent mechanism of water diffusion in the pentacene layer induces dipole-charge carrier interactions through the creation of energetic disorder. This results in long-term irreversible reduction of drain current.

4:06PM L19.00007 Controlling charge carrier injection in solution processed pentacene transistors by molecular engineering of the electrodes, SANGAMESHWAR RAO SAUDARI, Department of Materials Engineering, University of Pennsylvania, CHERIE KAGAN, Department of Electrical and Systems Engineering, University of Pennsylvania — We present the device performance of pentacene transistors fabricated from a solution deposited precursor. The bottom-contact pentacene transistors are fabricated by spin-coating N-sulfinylacetamidopentacene precursor followed by thermal conversion of the precursor into pentacene. Hole mobilities >0.1 cm2/Vs and Ion/Ioff > 105 are repeatedly achieved by this process. The metal-semiconductor interface in organic transistors plays a very important role in charge carrier injection and the overall device performance. Here we have treated the metal surface with self-assembled monolayers having different head and tail chemistries prior to pentacene precursor deposition to tailor the interfacial electronic properties. We correlate monolayer chemistry with device contact resistance and threshold voltage. These studies are used to fabricate devices with high mobility, high Ion/Ioff and low subthreshold swing. Device hysteresis and stability issues will also be presented.

4:18PM L19.00008 Infrared and Electro-Optic Properties of TIPS-Pentacene1, E.G. BITTLE, J.W. BRILL, J.E. ANTHONY, University of Kentucky — We will discuss new measurements of the infrared and electro-optic properties of thin crystals of trisopropylsilylhexylpentacene (TIPS) pentacene. As with THz studies of this class of materials, crystalline films were grown from saturated tetrahydrofuran solutions on a gold electrode mask. Square wave voltages were applied to the electrical contacts on the sample as well as a gate electrode below the sample, through an oxide dielectric. Changes in phonon frequencies were studied as functions of voltage, position between contacts, and frequency of applied voltage. The results are interpreted in terms of charge diffusion through the TIPS-pentacene crystals.

1This research was supported by NSF-DMR Grants 0801764 and 0400938.

4:30PM L19.00009 Crossover from recombination limited charge transport to mobility restricted charge transport in organic LED1, VLADIMIR PRIGODIN, ARTHUR EPSTEIN, Physics Department, Ohio State University, Columbus, OH 43210-1117 — The model of bipolar charge transport in organic semiconductors where the current solely is provided by e-h recombination (LEDs structures) is studied [1]. We have shown that depending on recombination rate there are two basic regimes of charge transport. For recombination rate above the critical value the current is space charge limited and the current as a function of recombination rate decreases with increasing the recombination rate. At recombination rate below the critical value the recombination takes place over the whole sample volume of sample and as a result the current is only contact limited. As a function of recombination rate the current increases with increasing recombination rate. Critical value for recombination rate depends on the thickness of sample, applied voltage and on both the hole and electron mobilities. [1] J.D. Bergeson et al., Phys. Rev. Lett. 100, 067201 (2008).

1Supported by NSF, DOE and AFOSR.

4:42PM L19.00010 Interface and bulk controlled charge transport in Pd/CuPc/Pd sandwich devices. CORNELIU COLESNICU, IVAN SCHULLER, University of California San Diego, La Jolla, CA 92093 — We present transport measurements in thin film devices of copper phthalocyanine sandwiched between palladium electrodes. The devices were grown in-situ using molecular beam deposition of phthalocyanine films with the thickness ranging between 30 and 600 nanometers. The I-V characteristics as a function of temperature and thickness exhibit two distinct regions - a low voltage Ohmic region with current proportional to the voltage and a high voltage region with a power law dependence. At low voltages the current shows an inverse power dependence on thickness, I ~ thickness^-n, with the exponent n > 2, suggesting that both the interfaces and the film control the transport mechanism. The temperature dependence of the current does not show a clear activated behavior, supporting the same conclusion. On the other hand, at high voltages the power-law exponent of the I-V decreases at lower thickness for constant temperature implying also that both the interfaces and the film may control the transport. Work supported by AFOSR.

4:54PM L19.00011 RC Transmission Line Characterization of Organic Semiconductors1, DANIEL LENSKI, ADRIAN SOUTHARD, MICHAEL S. FUHRER, Department of Physics and Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, USA — We have characterized thin films of organic semiconductors (pentacene and poly-3-hexylthiophene) using a 3-contact transmission line configuration, in which an AC voltage is applied between the thin film and the gate, and the phase and magnitude of the current are measured. We compare the results with those obtained from simultaneous DC measurement, and find good agreement in the sheet resistance in the ON state measured using the DC and transmission line techniques, indicating that the transmission line technique is useful for obtaining sheet resistance and mobility in the ON state. Near threshold, or at high frequencies and electric fields, we observe systematic deviations of the AC impedance from the DC values. We discuss these deviations in terms of the of frequency-dependent length scale probed by the transmission line technique, and how these measurements can shed light on the properties of the semiconductor materials as well as their interfaces with contacts and substrates.

1This work has been supported by the Laboratory for Physical Sciences.
5:06PM L19.00012 Organic field effect transistors having single wall carbon nanotubes electrodes  
FABIO CICOIRA1, MSE/Cornell University, CARLA M. AGUIRRE, PATRICK DESJARDINS, Genie Physique /Polytechnique Montreal, RICHARD MARTEL, Chemie/Universite de Montreal — Single Wall Carbon Nanotubes (SWCNTs) are of great interest as electrode materials in Organic Field Effect Transistors (OFETs). Thanks to their field emission properties, SWCNTs electrodes, in principle, are able to inject both electrons and holes into organics with low injection barriers, promoting tunneling injection. We present well recent present result on the electrical properties of OFETs using hairy SWCNTs electrodes (see Figure 1), where the CNTs are attached on the substrate by means of metallic Ti contact pads. Devices with SWCNTs electrodes show improved injection characteristics compared with devices using conventional metallic electrodes.

1 Also at CNR/IFN, Trento (Italy)

5:18PM L19.00013 Electrospun tin oxide/poly(3-hexylthiophene) nanofiber p-n diodes  
NICHOLAS PINTO, University of Puerto Rico - Humacao — Electrospinning is a simple technique used to prepare nanofibers of various materials, organic and inorganic. Some advantages of this method is that the nanofibers are orders of magnitude longer than that obtained via conventional means and it is easy to isolate individual nanofibers. We have used this technique to make nanoribbons of n-doped tin oxide (SnO2) and to make nanofibers of p-doped region-regular poly(3hexylthiophene) (P3HT) in air and within seconds. Several p–n junction nanodiodes were fabricated by crossing individual nanofibers of P3HT with individual nanoribbons of SnO2 during the electrospinning process and electrically characterized them at room temperature. The SnO2 nanoribbons were fabricated first by electrospinning a precursor of SnO2 and then sintering them at 700 C to convert it to SnO2 before crossing them with P3HT nanofibers. The devices show clear evidence of rectification in air and in vacuum with a turn-on voltage of ~0.4 V and with rectification ratios ~10. Exposure of the diode to UV light increases the on-state current, while removing the light restores the device to its original state making it suitable as a reusable UV light sensor as well.

3:06PM L20.00002 Patterns on the iridescent beetle, Chrysina gloriosa  
JUNG OK PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, VIVEK SHARMA, Department of Mechanical Engineering, Massachusetts Institute of Technology, MATIJA CRNE, School of Chemistry and Biochemistry, Georgia Institute of Technology, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology — The brilliant metallic color of a beetle Chrysina gloriosa has been known to occur due to selective reflectance from a cholesteric structure on the exoskeleton. The surface also appears to have hexagonally packed structures. Crystallographic concepts and Voronoï analysis were used to determine the degree of order in different regions of the beetle. Along the hexagons in the Voronoï diagram, many clustered pentagons and heptagons were observed due to the surface curvature, the number of pentagons was found to be higher than the number of heptagons. The cells appear yellow in the center surrounded by a green region with a yellow edge. Confocal microscopy was used to image the underlying structure, which was found to consist of concentric arcs on a surface of a shallow cone. The observed structures resemble the defects on a cholesteric phase with a free surface, and provide an interesting explanation of structural color development in beetles, along with inspiration for the design of chiral photonic structures.

3:18PM L20.00003 Frustrated self-assembly of dendron and dendrimer-based supramolecular liquid crystals  
RAFFAELE MEZZENGA, NADIA CANILHO, University of Fribourg, Switzerland, JANNE RUOKOLAINEN, Helsinki University of Technology, Finland, EDIS KASEMI, DIETER SCHLUETER, ETHZ, Switzerland, WON BO LEE, GLENN FREDRICKSON, UCSB, USA — A new inverted topological configuration is demonstrated both experimentally and theoretically for self-assembled dendron and dendrimer-based supramolecular liquid crystals in which the dendrons/dendrimers occupy the continuous domain and the ionically attached pendant chains are confined in discrete domains. All previous studies on dendrimer and dendron-based liquid crystals have reported normal liquid crystalle configurations in which the dendritic templates occupy discrete domains (in spherical or columnar phases) or continuous struts (in bicontinuous cubic phases), while the pendant chains occupy the continuous space-filling domain. These surprising results mandate a re-examination of the packing mechanisms for this important class of materials and open new routes to unique nanostructures of possible use in existing and emerging technologies. References: R. Mezzenga, J. Ruokolainen, N. Caniello, E. Kasemi, D.A. Schlüter, W.B. Lee, G. H. Fredrickson, Soft Matter, in press (DOI: 10.1039/b814972k)

3:30PM L20.00004 Hydrogen-Bonding Assisted Supramolecular Self-Assembly of Double Dis-otic Supermolecules  
JIANGJUN MIAO, LEI ZHU, Uconn — Symmetric double disotic supermolecules based on porphine (Py) and triphenylene (Tp), Py(Tp)4, have been successfully synthesized via PyBOP-catalyzed amidization reactions. The Tp moieties had either C5- or C12-arms, and the spacer linking between the central Py and peripheral Tp was either C8 or C10. Thermal properties of these supermolecules were studied by differential scanning calorimetry, and self-assembled crystalline and/or liquid crystalline textures were confirmed by polarized optical microscopy. For samples with C5-arms in Tp, only a crystal-melt transition was observed. X-ray diffraction (XRD) on shear-oriented samples showed that Py was crystalline and Tp formed columnar liquid crystal. For samples with C12-arms in Tp, sequential crystal-liquid crystal-isotropic melt transitions were observed. XRD results indicated that the crystalline unit cells were orthorhombic for all samples, and amide hydrogen-bonding was responsible for their supramolecular self-assembly.

3:42PM L20.00005 Glassy correlations in nematic elastomers  
BING LU, PAUL GOLDBART, University of Illinois at Urbana-Champaign, XIAOMING MAO, University of Pennsylvania — We address the physical properties of an isotropic melt or solution of nematogenic polymers that is then cross-linked beyond the vulcanization point. To do this, we construct a replica Landau theory involving a coupled pair of order—parameter fields: one describing vulcanization, the other describing local nematic order. Thermal nematic fluctuations, present at the time of cross-linking, are trapped by cross- linking into the vulcanized network. The resulting glassy nematic fluctuations are analyzed in the Gaussian approximation in two regimes. When the localization length is shorter than the thermal nematic correlation length, the nematic correlations are well captured as glassy correlations. In the opposite regime, fluctuations in the positions of the localized polymers partially wash out the glassy nematic correlations.
3:54PM L20.00006 Orientation distribution and process modeling of thermotropic liquid crystalline copolyester (TLCP) injection-moldings1, ROBERT BUBECK, Michigan Molecular Institute. JUN FANG, WESLEY BURGHARDT, Northwestern University, SUSAN BURGARD, Michigan Molecular Institute, DANIEL FISCHER, NIST — The influence of melt processing conditions upon mechanical properties and degrees of compound molecular orientation have been thoroughly studied for a series of well-defined injection molded samples fabricated from VECTRA (TM) A950 and 4,4'-dihydroxy-a-methylstilbene TLCPs. Fracture and tensile data were correlated with processing conditions, orientation, and molecular weight. Mechanical properties for both TLCPs were found to follow a “universal” Anisotropy Factor (AF) associated with the bimodal orientation states in the plaques determined from 2-D WAXS. Surface orientations were globally surveyed using Attenuated Total Reflectance – Fourier Transform Infrared (ATR-FTIR) spectroscopy and C K edge Near-Edge X-ray Absorption Fine Structure (NEXAFS). The results derived from the two spectroscopy techniques confirmed each other well. These results along with those from 2-D WAXS in transmission were compared with the results of process modeling using a commercial program, MOLDFLOW(TM). The agreement between model predictions and the measured orientation states was gratifyingly good.

1Research is supported by NSF Grant Nos. 0521771 and 0521823.

4:06PM L20.00007 In Situ X-ray Scattering Measurements and Polydomain Simulations of Molecular Orientation Development during Injection Molding of Liquid Crystalline Polymers. JUN FANG, WESLEY BURGHARDT, Northwestern University, ROBERT BUBECK, Michigan Molecular Institute — We report on a coordinated experimental/computational study of injection molding of commercial thermotropic LCPs. In situ synchrotron x-ray scattering, combined with a customized injection molding apparatus, is used to track development of molecular orientation during the mold filling process for a commercial LCP, Vectra A950, in two simple plaque mold geometries: square and T-shaped. Use of high brilliance undulator radiation at the Advanced Photon Source, coupled with a high speed CCD detector provides sufficient time resolution (~12 frames per second) to resolve the transient orientation dynamics during and following mold filling. In addition to in-situ scattering measurements, ex-situ 2-D wide angle X-ray scattering measurements are conducted on the same injection molded plaques. The experiments are complemented by process simulations performed using commercial mold filling software. A very close analogy between the Folgar-Tucker fiber orientation model and the Larson-Doi polydomain model for textured liquid crystalline polymers is exploited to allow for the first tests of Larson-Doi model predictions in injection molding processing.

4:18PM L20.00008 Dynamics and rheology of active polar liquid crystalline films, LUCA GIOMI, M. CRISTINA MARCHETTI, TANNIEMOLA B. LIVERPOOL — I will discuss the dynamical and rheological properties of active polar liquid crystalline films. Like active nematic films, active polar films undergo a dynamical transitions to spontaneously flowing steady states. Spontaneous flow in polar fluids is, however, always accompanied by strong concentration inhomogeneities or “banding” not seen in nematics. In addition, a spectacular property unique to polar active films is their ability to generate spontaneously oscillating and banded flows even at low activity. The oscillatory flows become increasingly complicated for strong polarity.

4:30PM L20.00009 Influence of nanorods on the properties of polymeric materials, GREGORY N. TOEPFERWEIN, ROBERT A. RIGGLEMAN, JUAN J. DE PABLO, University of Wisconsin — Nanoscopic additions, such as metallic nanoparticles or carbon nanotubes, can dramatically impact the mechanical properties of polymeric materials, such as the plateau modulus, which is intimately related to the entanglement length of the polymer. To explore the connection between nanocomposite configurations and the dynamic mechanical effects that are difficult to probe experimentally, due to challenges associated with sample preparation and particle dispersion, we have performed extensive Molecular Dynamics and Monte Carlo simulations of polymer nanocomposites with nanoparticles whose size, shape, and concentration have been varied systematically. Calculations of the entanglement network through primitive path analysis of these composites have enabled us to connect nanorod effects on the entanglement network structure and density to the system’s dynamic properties. The main outcome of our study is a better understanding of how inclusions alter entanglements and how those entanglements are magnified in macroscopic observables.

4:42PM L20.00010 Interactions between rod-like cellulose nanocrystals and xylan derivatives: A light scattering study, JAE HYUN SIM, Virginia Tech, KATRIN SCHWIKAL, THOMAS HEINZE, University of Jena, SHUPING DONG, MAREN ROMAN, ALAN ESKER, Virginia Tech — Interactions between rod-like cellulose nanocrystals and 2-hydroxypropyl-trimethylammonium (HPMA) xylan were investigated by polarized (DLS) and depolarized dynamic light scattering (DDLS). Cellulose nanocrystals were prepared by the controlled hydrolysis of black spruce pulp. Binary rod-like cellulose nanocrystal/water and ternary HPMA xylan/rod-like cellulose nanocrystal/water systems with different concentrations of cellulose nanocrystals were probed. Translational and rotational diffusion coefficients of cellulose nanocrystals in water are (4.8 ± 0.4) × 10−9 cm2/s and (526 ± 20) s−1, respectively, and calculated lengths and diameters for nanocrystals are comparable to those of cellulose whiskers from cotton. At high cellulose nanocrystal concentrations, DDLS studies in ternary systems provide translational and rotational diffusion coefficients. However, at low cellulose nanocrystal concentrations, DDLS studies of ternary systems do not yield rotational diffusion coefficients. This behavior is attributed to bridging between polymer chains that causes non-linear deviation on standard decay rate (Γ) versus scattering vector magnitude (q) plots.

4:54PM L20.00011 Polymerization-Enhanced Alignment Order in Carbon Nanotube Composites, HOWARD WANG, YAYONG LIU, NARANYAN DAS, Binghamton University, SUNY, KUNLUN HONG, GYULA ERES, DAVID URG, Oak Ridge National Laboratory — Polymer nanocomposites containing vertically aligned carbon nanotubes (VACNTs) have been synthesized via vacuum infiltration of monomers into confined VACNT arrays fabricated by in situ polymerization. The alignment order of VACNTs before and after polymerization has been quantitatively assessed using small angle neutron and x-ray scattering. The trend of continuous variation of alignment order along the height of VACNTs remains unaltered whereas the degree of order is enhanced upon polymerization. Polymerization-enhanced alignment order may assist preparing better carbon nanotube composites.

5:06PM L20.00012 Perylene diimide liquid crystals: A density functional study, JEVERSON ARANTES, Centro de Ciencias Naturais e Humanas, Universidade Federal do ABC, Santo Andre, SP, Brazil, MATHEUS LIMA, Institute of Fundamental Sciences, University of Auckland, New Zealand, GREGORY N. TOEPFERWEIN, ROBERT A. RIGGLEMAN, JUAN J. DE PABLO, University of Wisconsin, SUSAN BURGARD, Michigan Molecular Institute, DANIEL FISCHER, NIST — Perylene diimide PEBEE has been proposed, partially based on experimental observations. In this structural model, we’ve performed an ab initio calculations on the electronic structure of this material. Due to the strongly localized nature of the Oxygen atoms on the side chains, it is necessary to go beyond the standard LDA and GGA calculations. With the PBE0 approach, the electronic structure becomes in agreement with previous results. The tails of the molecular crystal not only is responsible for its structural conformation, but also can be used for tuning the electronic and optical properties of the material.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L21 DCMP FIAP: Semiconductors: Atomic Structure and Lattices
2:30PM L21.00001 ABSTRACT HAS BEEN MOVED TO J23.00011

2:42PM L21.00002 Bonding states of Cu atoms in superionic α-Cul phase. HIROAKI OSHIHARA, KAZUO TSUMURAYA, Meiji University, Japan — The fast migration of cations in solids is used for solid state battery. Therefore the mechanism of the migration is of importance for the development of new material. The superionic conductor Cul is zinc blend-type structure at low temperature and fluorite-type at high temperature. So the bonding between Cu and I atoms has been considered to be a covalent bonding. The peak positions and the asymmetrical peaks in the pair distribution functions between the Cu-Cu and Cu-I components have been remained to be explained in an experiment and a computational studies. We investigate the electronic states of Cu using the plane-wave based density functional calculation. We evaluate the charge and bonding states with Bader decomposition method. The stability of the Cu-Cu pairs in the conductor will be discussed using their binding energies.

2:54PM L21.00003 Non-equilibrium Phonons in CaWO₄: Issues for Phonon Mediated Particle Detectors. MADELEINE MSALL, Bowdoin College, TIMOTHY HEAD, DANIEL JUMPER, Abilene Christian University — The CRESST experiment looks for evidence of dark matter particles colliding with nuclei in CaWO₄. Using cryogenic bolometers sensitive to energy deposition ~ 10 keV with a few percent accuracy, California, Los Angeles, K. BELASHCHENKO, Dep. of Physics and Astronomy, Univ. of Nebraska-Lincoln — We have computed the temperature-phase diagram of EuO alloys by combining density functional theory in the generalized-gradient approximation with Hubbard U correction on f-orbitals with the regular decomposition method. The stability of the Cu-Cu pairs in the conductor will be discussed using their binding energies.

3:06PM L21.00004 Ultrafast anisotropic strain in semiconductors measured by x-ray diffraction. D.A. WALKO, Argonne National Laboratory, SOOHEYONG LEE, Korea Research Institute of Standards and Science, E.C. LANDAHL, DePaul University, D.A. ARMS, Argonne National Laboratory — We have used time-resolved x-ray diffraction to probe the non-uniaxial properties of impulsive strains in ultrafast laser-excited III-V semiconductors. Transient shifts of x-ray rocking curves due to the strains are measured from three Bragg reflections whose scattering vectors range from perpendicular to the surface to nearly in plane. Time-dependent strain ellipsoids are then constructed, with a temporal resolution under ~150 ps. We find that the strain consists not only of a longitudinal expansion along the surface normal, but it also includes slight compression along the transverse direction. We compare measurements for GaAs and InSb; their significant differences in electron diffusion rates allow us to distinguish between lattice and electronic effects. Supported by the U.S. Department of Energy.

3:18PM L21.00005 Using DFT-based Cluster Expansions to Study Oxygen Adsorption on Platinum and Gold (111) Surfaces. SPENCER MILLER, Carnegie Mellon University — We have studied oxygen adsorption on Platinum and Gold (111) surfaces using Density Functional Theory. We have investigated the sensitization on the number of configurations we can consider through DFT through the use of two-dimensional cluster expansions on DFT data, allowing for high energy calculations for any arbitrary surface. We have used the cluster expansion to study adsorption properties and phase behavior on the surface including simulated TPD experiments and atomistic thermodynamics phase diagrams which we compare to experimental behavior.

3:30PM L21.00006 Can a re do of field theory numerically speaking help in I - E CDW curve data analysis? ANDREW BECKWITH — Density wave physics has a plethora of current versus electrical field data from experimental measurements. The author presented in his PhD dissertation a way of giving a false vacuum interpretation of how current can be measured against the magnitude of an applied electric field in laboratory conditions. This article purports to re examine the feasibility of such modeling taking into account Dr. Fred Cooper’s work on a time averaging scheme for phi to the fourth power field theory as could be applied to modified wash board potentials.

3:42PM L21.00007 Temperature-composition phase diagrams of Gd-doped EuO and EuS. JOONHEE AN, Dep. of Physics and Astronomy, Univ. of Nebraska-Lincoln, S. BARABASH, Dep. of Materials Science and Engineering, Univ. of California, Los Angeles, K. BELASHCHENKO, Dep. of Physics and Astronomy, Univ. of Nebraska-Lincoln. We have computed the temperature-phase diagram of EuO and GdO alloys by combining density functional theory in the generalized-gradient approximation with Hubbard U correction on f-orbitals with the regular cluster expansion and Monte-Carlo approach. The cluster expansion fit has been performed with varying numbers of distinct cluster types until the formal cross-validation score is minimized. Our results indicate that (i) pair interactions are relatively stronger than other cluster types, (ii) The pair terms are attractive for direct interactions between cations and repulsive for indirect interactions through anions, and (iv) the calculated convex hull is asymmetric about x=0.5, displaying more deep ground states in Eu-rich regions than in Gd-rich regions. The symmetry of the convex hull may relate relative instability of Gd-rich compounds, as was shown by previously-reported experimental difficulties to make Gd-rich compounds. A comparison with a similar binary system - sulfur replacing oxygen - is made, showing that both oxides and sulphides are dominated by deformation interaction.

3:54PM L21.00008 Low energy metastable states and immiscibility in (SiC)_{1-x}(AlN)_{x}. BENJAMIN BURTON, NIST, AXEL VAN DE WALLE, California Inst. of Technology, ALBERT DAVYDOV, NIST, VICTOR VINOGRAD, University of Frankfurt, Germany — A cluster expansion Hamiltonian was fit to VASP/PAW calculated supercell formation energies, \Delta E_I, and first principles based phase diagrams (miscibility gaps) were calculated for the wurzite-structure pseudobinary system SiC_{1-x}AlN_{x}. An unusually wide range of 3 \leq E_I \leq 125 \text{kJ/mole MX} (M= Al, Si; X = N, C) was calculated and all supercells with \Delta E_I \leq 8 \text{kJ/mole} exhibited characteristic (SiC)_{m}(AlN)_{n} crystallography, in which (SiC)_{m} indicates m SiC-double layers \perp to the hexagonal c-axis, and similarly for (AlN)_{n}. The prediction of (SiC)_{m}(AlN)_{n} low-energy metastable states, may explain why one can synthesize SiC_{1-x}AlN_{x} films, or single crystals of arbitrary bulk composition, in spite of the very strong tendency toward immiscibility. Specifically, one expects that metastable films or single crystals will be dominated by a disordered stacking of SiC- and AlN-double layers.

4:06PM L21.00009 Alloy Stabilized Wurtzite Ground State Structures of Zinc-Blende Semiconducting Compounds. HONGJUN XIAO, SUHUAI WEI, National Renewable Energy Laboratory, SHIYOU CHEN, XINGAO GONG, Surface Science Laboratory and Department of Physics, Fudan University, China — Although the ground state structures of zinc-blende (ZB) alloys have been extensively studied, the knowledge of the ground state structures of wurtzite (WZ) alloys remains incomplete. Here, the ground state structures of the A_B_{1-x}C WZ alloys with \( x = 0, 0.25, 0.5, \) and 0.75 are revealed by a ground state search using the valence-force field model and density-functional theory total energy calculations. It is shown that the ground state WZ alloy always has a lower strain energy and formation enthalpy than the corresponding ZB alloy. Therefore, we propose that the WZ phase can be stabilized through alloying. This novel idea is supported by the fact that the WZ AlP_{0.25}Sb_{0.5}, AlP_{0.75}Sb_{0.25}, ZnS_{0.5}Te_{0.5}, and ZnS_{0.75}Te_{0.25} alloys in the lowest energy structures are more stable than the corresponding ZB alloys. To our best knowledge, this is the first example where the alloy adopts a structure distinct from both parent phases.
4:18PM L21.00010 First-principles thermodynamic theory of phase transition mechanisms in Ge$_2$Sb$_2$Te$_5$.

4:30PM L21.00011 Atomistic origins of the phase transition mechanism in Ge$_2$Sb$_2$Te$_5$.


4:54PM L21.00013 Crystal and electronic structure of quaternary chalcogenide semiconductors.

5:06PM L21.00014 The electronic structures and structural properties of the amorphous Ge$_2$Sb$_2$Te$_5$.

5:18PM L21.00015 Molecular dynamics study on volume dependence of atomic and electronic structure in amorphous Ge$_2$Sb$_2$Te$_5$.

Tuesday, March 17, 2009 2:30PM - 5:30PM –
Session L22 GMAG DMP FLAP: Focus Session: Spin-Orbit Effects in Semiconductors

2:30PM L22.00001 ABSTRACT WITHDRAWN –
4:06PM L22.00007 Spin-orbit control of magnetization and electrical detection of current-induced spin polarization. MASON OVERBY, ALEX CHERNYSHOV, LEONID ROKHINSON, Purdue University, XINYU LIU, JACEK FURDYNA, Notre Dame University — The success of future spintronic devices relies on the efficient control and detection of spin polarization. Extrinsicly polarized currents, injected from ferromagnetic materials, can interact with magnetic domains and initiate domain rotation. Alternatively, spin polarization can be generated intrinsically via relativistic coupling of spin to the momentum of charge carriers, known as spin-orbit interaction (SO). While the use of SO for electrostatic control of polarization forms the basis of various theoretical device concepts, SO control of magnetization has not been realized experimentally. Here we demonstrate that magnetization can be reversibly manipulated by intrinsically polarized currents in ferromagnetic semiconductors with strong SO coupling. The system under consideration is a two-dimensional electron gas (2DES) that is present at the interface of a heterostructure due to modulation doping. Within this approach, we study the coupling between spin and charge and we determine the charge (spin) profile induced by a non-uniform, periodic spin (charge) density in the presence of the external electric field. We determine the optimal range of parameters for observing the spin-charge coupling effects.

3:42PM L22.00005 Magneto-transport in high mobility n-InSb/InAlSb quantum wells1, W.R. BRANFORD, A.M. GILBERTSON, Imperial College, L.F. COHEN, M. FEARN, P.D. BUCKLE, L. BUCKLE, QinetiQ Malvern — The inherent large spin-orbit (SO) coupling InSb quantum wells (QWs) is expected to result in sensitive tunability of the Rashba effect with electric field. The strength of the SO coupling can be extracted from measurements of weak anti-localisation (WAL) and from the beating of Shubnikov-de Haas (SdH) oscillations [1]. We have investigated these phenomena and report magneto transport measurements from a range of InSb/InAlSb QWs with varying carrier density n and mobility μ. It is shown that the inherent large Zeeman splitting combined with inhomogeneous level broadening means that beating in the SdH oscillations in InSb QWs are rarely observed. However, her we show that in InSb/InAlSb QWs, n can be modulated using a gate electric field from 1.15 < n < 3.3x10^{11} cm^{-2} with 13 < μ < 38 mV−1 cm−1 and that under certain conditions weak beating effects can be observed which are attributable to the Rashba effect. Extracted values of the Rashba parameter from beating [2], WAL and k.p modelling [3] is discussed. [1] V.A.Guzenko et al., PRB 76 (16), 165301 (2007) [2] G.Engels et al., PRB 55 (4), R1958 (1997) [3] A.M.Gilbertson et al., PRB 77 (16), 165335 (2008)

1Research supported by UK EPSRC.

3:54PM L22.00006 Diffusive spin-charge dynamics in an external electric field, TUDOR-DAN STANESCU, BRANDON ANDERSON, VICTOR GALITSKI, University of Maryland — We study the dynamics of a spin density injected into a two-dimensional electron system with generic spin-orbit interactions. We generalize the spin-charge diffusion equation formalism by including the effects of a uniform electric field. Within this approximation, we study the coupling between spin and charge and we determine the charge (spin) profile induced by a non-uniform, periodic spin (charge) density in the presence of the external electric field. We determine the optimal range of parameters for observing the spin-charge coupling effects.

3:06PM L22.00002 Pure spin current pump in a quantum channel with both Rashba and Dresselhaus effects, CHIA-HUI LIN, RCAS, Academia Sinica, CHI-SHUNG TANG, National United University, Taiwan, YIA-CHUNG REN, RCAS, Academia Sinica, Taiwan — We demonstrate a spin pump to generate pure spin current of tunable intensity and polarization in the absence of charge current. The system under consideration is a two-dimensional electron gas (2DEG) that is present at the interface of a heterostructure due to modulation doping and has intrinsic static Rashba and Dresselhaus spin-orbit interactions. The pumping functionality is achieved by means of an ac gate voltage that modulates the Rashba constant dynamically in a local region of a quantum channel in which both the static Rashba and Dresselhaus spin-orbit interactions are taken into account. The spin-resolved Floquet scattering matrix formalism is applied to our system. Based on the Floquet theorem, this formalism provides an exact and nonperturbative solution to the time-periodic Schrodinger equation in the mesoscopic system. Because the time-dependent spin-orbit interaction couples two spin polarizations and all sidebands together, analytic expression for the sideband dispersion is not feasible. Thus, we determine the sideband dispersion relation numerically by solving the Schrodinger equation in a nearly complete basis with the spatial inhomogeneity handled by matching boundary conditions region by region. The Floquet scattering matrix gives a coherent solution that goes beyond the adiabatic regime.

3:18PM L22.00003 Mesoscopic fluctuations in the spin-electric susceptibility due to Rashba spin-orbit interaction, MATHIAS DUCKHEIM, DANIEL LOSS, Department of physics, University of Basel — Spin-orbit interaction enables the control of the spin with electric fields in non-magnetic semiconductors. The orbital transport processes generating the internal fields that are necessary for this control of spin are non-local and mesoscopic. We investigate mesoscopic fluctuations in the spin polarization generated by a static electric field and by Rashba spin-orbit interaction in a disordered 2D electron gas. In a diagrammatic approach we find that the out-of-plane polarization — while being zero for self-averaging systems — exhibits large sample-to-sample fluctuations which are shown to be within experimental reach. We evaluate the disorder-averaged variance of the susceptibility and find its dependence on magnetic field, spin-orbit interaction, dephasing, and chemical potential difference. [M. Duckheim and D. Loss, Phys. Rev. Lett. (in print), arXiv:0805.4145v1]

3:30PM L22.00004 Spin-orbit coupling effects and the angular dependence of the tunneling anisotropic magnetoresistance1, ALEX MATOS-ABIAGUE, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We consider a tunnel junction in which one of the electrodes is ferromagnetic. Based on general properties and symmetry considerations, we develop a phenomenological model in which the anisotropy of the tunneling magnetoresistance with respect to the magnetization orientation of the ferromagnet originates from the spin-orbit interaction. The model reveals how the symmetry and angular dependence of the tunneling anisotropic magnetoresistance (TAMR) are determined by the form of the spin-orbit coupling field (SOCF), independently of the specific details of the system. We investigate the particularly important cases in which the SOCF is of Bychkov-Rashba and/or Dresselhaus type and obtain angular dependences which are in good agreement with available TAMR measurements. We also predict new forms of the angular dependence of the TAMR by exploring different geometric configurations.

3:24PM L22.00001 Spin-orbit interaction in low dimensional InSb/InAlSb systems, TUDOR-DAN STANESCU, RCAS, Academia Sinica, CHI-SHUNG TANG, National United University, Taiwan — Low temperature magnetotransport measurements were performed on high mobility InSb/InAlSb two dimensional electron systems (2DES) and quasi-1D wires fabricated from the 2DES. Anti-localization dominates the magnetoresistance in low applied magnetic fields; hence the spin-orbit interaction is sensitive to the electron spin and phase coherence lengths in the structures. Measurements of the low field magnetoresistance over temperature demonstrate that the antilocalization phenomena persists to temperatures above ~20 K in the quasi-1D wires, whereas antilocalization is not observed above ~15 K in the unpatterned 2DES. The extracted spin coherence lengths, obtained from fitting the magnetoresistance curves to localization theory, show only weak temperature dependence. Therefore, phase coherence appears to dominate the temperature dependence of antilocalization in the low dimensional InSb/InAlSb systems. (NSF DMR-0618235, DOE DE-FG02-08ER46532, NSF DMR-0520550)
4:30PM L22.00009 Full-zone spin-splitting for electrons and holes in bulk GaAs and GaSb
JUN-WEI LUO, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — The spin-orbit interaction — a fundamental electronic force — is equivalent to an effective magnetic field intrinsic to crystals, leading to band spin-splitting for certain k-points in sufficiently low-symmetry structures. This (Dresselhaus) splitting has usually been calculated at restricted regions in the Brillouin-zone via small-wavevector approximations (e.g., k·p). We provide a full-zone description of the Dresselhaus splitting in zinc-blend semiconductors by using pseudopotentials, empirically corrected to rectify LDA errors by fitting GW results at a few frequencies. We find that (i) The largest spin-splitting occurs along the [110] direction, not the [110] direction as previously thought based on limited view of the Brillouin zone; (ii) the spin-splitting of the upper valence band VB1 is comparable to that of the next two valence bands VB2 and VB3. This has been previously overlooked due to the expectation that the largest spin-splitting will occur along the [110] direction; (iii) The spin-splitting pattern of each band is orthogonal to each other.

1 Funded by DOE-SC-BES-MSED under Contract No. DE-AC36-08GO28308 to NREL.

4:42PM L22.00010 Controlling the persistent spin helix with strain induced spin-orbit coupling
LUYI YANG, Lawrence Berkeley National Laboratory and University of California Berkeley, JAKE KORALEK, Lawrence Berkeley National Laboratory, JOE ORENSTEIN, Lawrence Berkeley National Laboratory and University of California Berkeley, ANDREI BERNEVIG, Princeton University, SHOUCHENG ZHANG, Stanford University, SHAWN MACK, DAVID ANSCHALOM, Center for Spintronics and Quantum Computation, University of California Santa Barbara — We use transient spin grating spectroscopy to study the persistent spin helix (PSH) state of the 2D electron gas. The PSH is a meta-stable helical spin density wave that emerges as a result of increased symmetry when the Rashba and Dresselhaus spin-orbit coupling terms are balanced, and which offers great promise as a means of controlling large ensembles of spins. We demonstrate that the spin-orbit symmetry, and the PSH dynamics, can be manipulated in-situ by the application of uniaxial strain. This strain induces spin-orbit coupling with precisely the same symmetry as the Rashba term, allowing us to effectively tune the Rashba/Dresselhaus ratio in a single sample. This work is supported by DMSE office of BES-DOE, NSF, MARCO, ASE and CNID.

5:45PM L22.00011 The precessing persistent spin helix in a magnetic field
RUNDONG LI, Stanford University, JING WANG, Stanford University, SHOUNG CHUNG ZHANG, Stanford University — While the spin-orbit interaction is useful for manipulating the electron spin, it could also cause spin decoherence. A Persistent Spin Helix (PSH) with infinite life time has been predicted [B. A. Bernevig et al., Phys. Rev. Lett. 97, 236601 (2006)], for 2D quantum wells with equal strength of Rashba and Dresselhaus spin-orbit coupling. This effect results from the spin SU(2) symmetry of electrons, which makes the spin density at a finite wave vector conserved. The PSH was later observed in the transient spin grating (TSG) experiment [C. P. Weber et al., Phys. Rev. Lett. 98, 076604 (2007)], where the spin density wave is pumped and its decay in the time domain is probed optically. In this work we propose measuring the PSH with an in-plane magnetic field and spin injection with alternating polarization. We derive and solve the drift-diffusion equation for the spin density and find that the persistence of the spin injection is the same as the Larmor frequency, a great enhancement of the diffusion length and the amplitude of the spin oscillation should be observed, giving rise to a precessing PSH.

5:06PM L22.00012 Theory of Electron Spin Relaxation in ZnO
NICHOLAS HARMON, WILLIAM PUTIKKA, Ohio State University, ROBERT JOYNT, University of Wisconsin — Doped ZnO is a promising material for spintronics applications. For such applications, it is important to understand the spin dynamics and particular the spin relaxation times of this II-VI semiconductor. The transverse spin lifetime $T_\perp$ has been measured by optical orientation experiments, and it shows a surprising non-monotonic behavior with temperature. We explain this behavior by invoking spin exchange between localized and extended states. Interestingly, the effects of spin-orbit coupling are by no means negligible, in spite of the relatively small valence band splitting. This is due to the wurtzite crystal structure of ZnO. Detailed analysis allows us to characterize the impurity binding energies and densities, showing for the first time that optical orientation experiments can actually be used as a characterization tool for semiconductor samples.


1 Financial support was provided by the National Science Foundation, Grant Nos. NSF-ECS-0523918 (NH and WP) and NSF-ECS-0524253 (RJ).

5:18PM L22.00013 Effect of Induced Spin-orbit Coupling in Cold Atomic Gas
XIANG-JUN LIU, MARIO F. BORUNDA, XIN LIU, JAIRO SINOVÁ, Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA, JAIRO SINOVÁ’S GROUP AT TAMU TEAM — Spin-orbit (SO) coupling effect in superfluids has emerged in the solid-state community as a very active field of research, fueled in part by the field of spintronics, e.g. spin current injection with spin Hall effect [1]. Recently, new schemes are developed to generate the SO interaction in cold atoms [2], which opens new possibilities in studying Spintronics in atomic systems. Here we shall report our recent proposal of SO coupling effects in Fermi atomic systems via optical method [3]. The induced SO coupling can be of the Dresselhaus and Rashba type with a Zeeman term. We show that the optically induced SO coupling can lead to a spin-dependent effective mass under proper condition, with one of them able to be tuned between positive and negative effective masses. As a direct observation we show that in the expansion dynamics of the atomic cloud the initial atomic cloud can split into two or four clouds depending on the effective mass regimes. Reference: [1] S. Murakami et al., Science 301, 1348 (2003); J. Sinová et al., Phys. Rev. Lett. 92, 126603 (2004). [2] X.-J. Liu et al., Phys. Rev. Lett. 98, 026602 (2007); S.-L. Zhu et al., ibid, 97, 240401 (2006); T. D. Stancu et al., ibid, 99, 110403 (2007). [3] X.-J. Liu, M. F. Borunda, X. Liu, J. Sinova, submitted to PRL for publication, arxiv:0808.4137 (2008).

1 Principal Investigator

Tuesday, March 17, 2009 2:30PM - 5:30PM – Session L23 DCMP FIAP: Fractional Quantum Hall Effect, Bilayers 325

2:30PM L23.00001 Different Signatures of the Total Filling Factor 1 State
LARS TIEMANN, YOUNGSOO YOON, STEFAN SCHMULT, MAIK HAUSER, WERNER DIETSCHE, KLAUS VON KLITZING, Max-Planck Institute for Solid State Research — Bringing two 2-dimensional electron systems in close proximity can yield a correlated state as the electrons will experience the presence of the neighboring system. At the individual filling factors of 1/2 this leads to a new double-layer ground state as positive and negative charges from opposite layers couple to excitons. Many remarkable properties were found such as vanishing Hall and longitudinal resistances in the counterflow configuration [1], a resonantly enhanced zero bias tunneling peak [2], and more recently, a critical DC tunneling current and vanishingly small interlayer resistances in DC measurements [3]. We will show how it is possible to combine the results of these three different measurements into a consistent picture. Under certain conditions it is possible to exceed the critical currents but still observe a minimum at total filling factor 1 in the counterflow configuration.

2:42PM L23.00002 Valley polarization and the polarization mass of composite fermions around $\nu = 3/2$, MEDINI PADMANABHAN, TAYFUN GOKMEN, MANSOUR SHAYEGAN, Dept. of Electrical Engineering, Princeton University, Princeton, NJ 08544 — In two-dimensional electron systems confined to AlAs quantum wells, composite fermions (CFs) around $\nu = 3/2$ are known to possess a valley degree of freedom [1]. The relative occupation of the valleys can be controlled via the application of uniaxial, in-plane strain. In this study, we measure the strain needed to completely valley-polarize the various fractional quantum Hall states around $\nu = 3/2$ as a function of density and compare our results to the theory explaining the complete spin-polarization of CFs in GaAs [2]. While the theory predicts it to be a constant, the energy needed for complete valley-polarization in units of the Coulomb energy is experimentally found to increase with increasing density. Translating this to the language of the 'polarization mass' for the CFs [2], we find an absence of the theoretically expected $\sqrt{B}$ dependence for the polarization mass. [1] N. C. Bishop et al., Phys. Rev. Lett. 98, 266404 (2007) [2] K. Park and J. K. Jain, Phys. Rev. Lett. 80, 4237 (1998)

2:54PM L23.00003 Clausius-Clayperon relation for onset of the coherent $\nu = 1$ phase in bilayer quantum Hall systems, YUE ZOU, GIL REFAEL, JAMES EISENSTEIN, Department of Physics, California Institute of Technology, Pasadena, CA 91125, USA, ADY STERN, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100 — A bilayer system of two-dimensional electron gases in a perpendicular magnetic field exhibits extremely rich phenomena. At total filling factor $\nu = 1$, as one increases the layer separation, the bilayer system goes from an interlayer coherent exciton condensed state to an incoherent phase of two decoupled composite fermion Fermi liquids. Many question still remain as to the nature of the transition between these two phases. Recent experiments investigated the phase boundary as a function of both in plane magnetic field and density imbalance. We compare these experimental results, e.g., the curvature of the phase boundary, with respect to the interlayer density imbalance, with a theoretical calculation based on the assumption that there is a direct first order transition between the two phases.

3:06PM L23.00004 Quantum Hall Bilayer in a Periodic Potential, GANPATHY MURTHY, University of Kentucky, JIANMIN SUN, HERBERT FERTIG, Indiana University — Disorder is known to be central to the interlayer density imbalance, with a theoretical calculation based on the assumption that there is a direct first order transition between the two phases. We compare these experimental results, e.g., the curvature of the phase boundary, with respect to the interlayer density imbalance, with a theoretical calculation based on the assumption that there is a direct first order transition between the two phases.

3:18PM L23.00005 Piezoresistance and Metal Insulator Transition of Composite Fermions at $\nu = 3/2$, TAYFUN GOKMEN, MEDINI PADMANABHAN, MANSOUR SHAYEGAN, Dept. of Electrical Engineering, Princeton University, Princeton, NJ 08544 — In the composite fermion (CF) picture, at the Landau level filling factor $\nu = 3/2$ the particle-flux CF quasi-particles are analogous to electrons at zero perpendicular magnetic field. Here we report piezoresistance measurements of CFs at $\nu = 3/2$ in AlAs quantum wells. In this system, the electrons occupy two conduction band valleys with elliptical Fermi contours, and the valley occupation of electrons can be controlled via the application of uniaxial, in-plane strain. The system's response to strain at $\nu = 3/2$ is qualitatively very similar to that of the electrons at zero perpendicular magnetic field, and consistent with the picture of CFs with a valley degree of freedom. Temperature dependent studies also show that CFs, like their counterpart electrons, go through a metal-insulator transition as they become valley polarized.

3:30PM L23.00006 Composite Fermion signature in the single particle spectrum of the fractional quantum Hall system, RAY ASHOORI, OLIVER DIAL, MIT, LOREN PFIEFFER, KEN WEST, Bell Laboratories, Alcatel-Lucent — Using time domain capacitance spectroscopy we measure the single particle spectrum of the fractional quantum Hall system. The very high energy resolution of the technique (limited ultimately only by sample temperature) allows us to uncover the existence of new spectral features. Among these is a sharp line that crosses the Fermi level at filling factor $\nu = 1/2$. The structure is consistent with the composite Fermion Landau fan, allowing measurement of the composite Fermion mass. Observation of this feature allows us to study the composite Fermion mass as a function of magnetic field and filling fraction.

3:42PM L23.00007 Quasiparticles in the tunneling spectrum of the fractional quantum Hall system, OLIVER DIAL, RAYMOND ASHOORI, MIT, LOREN PFIEFFER, KEN WEST, Bell Laboratories, Alcatel-Lucent — Despite the central role that the tunneling (or single-particle) particle density of states (TDOS) plays in our theories of many-body systems, it has proven a difficult quantity to access experimentally in two dimensional electron systems. We have developed a technique, time domain capacitance spectroscopy, which allows measurement of the TDOS over a range of 30 meV centered about the Fermi surface, revealing the detailed and beautiful structure present in these systems far from the Fermi energy. With increased sample quality and higher magnetic fields, we see the emergence of the fractional quantum Hall effect in the TDOS along with negative compressibility and chemical potential jumps associated with several fractions. Most strikingly, we also observe a number of new, sharp quasiparticle lines far from the Fermi energy. The dependence of the quasiparticle energies on density allows us to identify different fractional quasiparticles as well as estimate emergent effective quasiparticle masses. These high energy spectral features shed new light on the highly correlated fractional ground state, as well as the nature of the state near $\nu = 1$.

3:54PM L23.00008 Quantum Hall States at filling $\nu = k + \frac{2}{2k+\nu}$, WAHEB BISHARA, GREGORY FIETE, California Institute of Technology, CHETAN NAYAK, UCSB, Microsoft Research Station Q — We study the $\nu = k/2 + 1/2k$ quantum Hall states which are particle-hole conjugates of the $\nu = k/2$ Read-Rezayi states. We find that equilibration between the different modes at the edge of such a state leads to an emergent SU(2)$_0$ algebra in the counter-propagating neutral sector. Heat flow along the edges of these states will be in the opposite direction of charge flow. In the $k = 3$ case, which may be relevant to $\nu = 2 + \frac{2}{3}$, the thermal Hall conductance and the exponents associated with quasiparticle and electron tunneling distinguish this state from competing states such as the hierarchy/Jain state.

4:06PM L23.00009 Phase diagram for bilayer quantum Hall effect at total filling $\nu_\perp = 5$, CHUNTAI SHI, SHIVAKUMAR JOLAD, Department of Physics, The Pennsylvania State University, NICOLAS REGNAULT, Laboratoire Pierre Aigrain, ENS, CNRS, France, JAINENDRA JAIN, Department of Physics, The Pennsylvania State University — There has been much interest in bilayer quantum Hall systems at total filling $\nu_\perp = 1$, which exhibit excitonic superfluidity at small separations and two uncoupled composite fermion Fermi seas at large separations. We evaluate the phase diagram of the bilayer quantum Hall effect at total filling $\nu_\perp = 5$, neglecting interlayer tunneling and spin fluctuations, which is expected to be a bilayer excitonic superfluid at small separations and two uncoupled 5/2 FQHE states at large separations. Based on a combination of variational and exact diagonalization (for up to 20 electrons) studies, we estimate that the transition between these states occurs at a layer separation of approximately one magnetic length, independent of the individual layer thickness. The composite fermion Fermi sea is not found to be relevant for any parameters.
4:18PM L23.00010 How universal is the fractional quantum Hall edge physics?, SHIVAKUMAR JOLAD, The Pennsylvania State University, DIPTIMAN SEN, Indian Institute of Science, JAINENDRA JAIN, The Pennsylvania State University — We report on study of edge excitations of fractional quantum Hall states at filling factors \( \nu = 1/3 \) and \( \nu = 2/5 \). By considering the restricted basis of composite fermion wave functions, which is very accurate for the low energy eigenstates, we are able to diagonalize systems with up to 54 particles which allows us to make extrapolations to the thermodynamic limit. In a model with neutralizing positive jellium background disk at a distance \( d \), we find that edge reconstruction is generic, occurring even when the electron and the background disks coincide. We also test the postulated form for the electron field operator of the effective field theory approach for the fractional edge and find it to be inconsistent with our microscopic calculations. Implications of our results for the observed non-universality of the edge exponent will be discussed.

4:30PM L23.00011 A universal molecular description for the spectra of bosons and fermions in the lowest Landau level 1. CONSTANTINE YANNOULEAS, UZI LANDMAN, Georgia Institute of Technology — We show that both the ground and excited states in the LLL spectra of small systems can be expressed as linear superpositions of appropriate rovibrational molecular trial functions, akin to the rotating-electron-molecule functions introduced earlier. Thus the nature of strong correlations in the lowest Landau level reflects the spontaneous emergence of intrinsic point-group symmetries associated with rotations and vibrations of molecules of localized particles arranged in concentric polygonal-ring configurations. The present molecular picture is valid for both bosons and fermions. We stress its validity and superiority for low (as well as high) angular momenta, where “quantum-fluid” trial functions of a markedly different nature (including Laughlin, composite-fermion, and Pfaffian ones) have been assumed to apply.

4:42PM L23.00012 Origin of chiral p-wave pairing in even-denominator fraction quantum Hall effect., YUAN-MING LU, Department of Physics, Boston College, YUE YU, Institute of Theoretical Physics, Chinese Academy of Sciences, ZIQIANG WANG, Department of Physics, Boston College — We show that gauge field fluctuations in the composite fermion field theory can be exactly integrated out using a non-unitary transformation. An instantaneous statistical interaction is induced which makes the Fermi sea unstable to chiral p-wave pairing. We show that the paired state is a Moore-Read Pfaffian and discuss the effects of Coulomb interaction in connection to even-denominator fractional quantum Hall effect.

4:54PM L23.00013 Pinning mode integer quantum Hall Wigner crystal of skyrmions, HAN ZHU, Princeton Physics; NHMFL, G. SAMBANDAMURTHY, Y.P. CHEN, P.-H. JIANG, NHMFL/FSU; Princeton EE, L.W. ENGEL, NHMFL/FSU, D.C. TSUI, Princeton EE, L.N. PFEIFFER, K.W. WEST, Bell Labs — Just away from integer Landau level (LL) filling factors \( \nu \), the dilute quasi-particles/holes at the partially filled LL form an integer-quantum-Hall Wigner crystal, which exhibits microwave pinning mode resonances [1]. Due to electron-electron interaction, it was predicted that the elementary excitation around \( \nu = 1 \) is not a single spin flip, but a larger-scale spin texture, known as a skyrmion [2]. We have compared the pinning mode resonances [1] of integer quantum Hall Wigner crystals formed in the partly filled LL just away from \( \nu = 1 \) and \( \nu = 2 \), in the presence of an in-plane magnetic field. As an in-plane field is applied, the peak frequencies of the resonances near \( \nu = 1 \) increase, while the peak frequencies below \( \nu = 2 \) show negligible dependence on in-plane field. We interpret this observation as due to a skyrmion crystal phase around \( \nu = 1 \) and a single-hole Wigner crystal phase below \( \nu = 2 \). The in-plane field increases the Zeeman gap and causes shrinking of the skyrmion size toward single spin flips. [1] Yong P. Chen et al., Phys. Rev. Lett. 91, 016801 (2003). [2] S. L. Sondhi et al., Phys. Rev. B 47, 16 419 (1993); L. Brey et al., Phys. Rev. Lett. 75, 2562 (1995).

5:06PM L23.00014 Observation of a Fractional Quantum Hall State at \( \nu = 1/4 \) in a Single Wide GaAs Quantum Well, DWIGHT R. LUHMAN, Department of Electrical Engineering Princeton University, W. PAN, Sandia National Laboratories, D.C. TSUI, Department of Electrical Engineering Princeton University, L.N. PFEIFFER, K.W. BALDWIN, K.W. WEST, Bell Laboratories — We have preformed low temperature (\( T = 35 \) mK) transport measurements using a 50 nm high-quality GaAs quantum well with an electron density of \( n_{e} = 2.55 \times 10^{11} \) cm\(^{-2} \) and a mobility of \( \mu \approx 10^7 \) cm\(^2\)/Vs. Magnetic fields up to \( B = 15 \) T were used to reach filling factor \( \nu = 1/4 \). With the sample situated perpendicular to the applied magnetic field, the diagonal resistance displays a kink at \( \nu = 1/4 \). When the sample is tilted to an angle of \( \theta = 30.3^\circ \), a clear minimum in the diagonal resistance and plateau in the Hall resistance are present at \( \nu = 1/4 \), indicating a fractional quantum Hall state at \( \nu = 1/4 \) in this sample. Several possibilities regarding the origin of this state will also be discussed.

5:18PM L23.00015 Charge-density wave formation in interacting two-dimensional electronic systems with Landau level mixing, PETER SMITH, MALCOLM KENNEDY, Simon Fraser University — Anisotropic transport in half-filled Landau levels has been explained in terms of charge-density wave (CDW) formation. We use the Hartree-Fock approximation to study the influence of electron-electron interactions and Landau level mixing on the formation of CDWs in two-dimensional electron and hole systems. For the situation of two nearly degenerate eigenstates, we construct a Landau free-energy theory appropriate for competing order parameters that allows for both striped and triangular CDW formation. We find the possibility of coexisting CDW ordering in the two states, along with possible hysteretic behaviour. This physics might be realized using an external parameter such as spin-orbit coupling to tune states into near degeneracy.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L24 DMP: Focus Session: Electronic Properties of Nanotubes 326

2:30PM L24.00001 Strongly Correlated Electron Phenomena in Carbon Nanotubes, MARC BOCKRATH, California Institute of Technology — In this talk I will discuss our recent results demonstrating strongly correlated electron behavior in ultra-clean carbon nanotube quantum dots. Specifically, we have observed one-dimensional (1D) Wigner crystal behavior of dilute holes in semiconducting nanotubes, finding three distinct regimes of spin and valley quantum number ordering as the charge density and axial magnetic field are varied. The boundaries between the regimes in density and magnetic field are well-described by the theory of Levitov and Tsvelik for a narrow-gap Luttinger liquid. In the second part of the talk I will present results showing that the electrons in nominally metallic nanotubes comprise a 1D Mott insulator. This indicates that carbon nanotubes are never truly metallic, in agreement with theoretical predictions that account for Umklapp scattering at half-filling due to electron-electron interactions. Using inelastic cotunneling spectroscopy, we also observe neutral electronic excitations within the gap, yielding an additional signature of the Mott insulating state. Our results demonstrate nanotubes’ promise for studying a variety of tunable correlated electron phenomena in 1D.
3:06PM L24.00002 Relaxation and dephasing in a two-electron $^{13}$C nanotube double quantum dot , HUGH CHURCHILL, FERDINAND KUEMMETH, JENNIFER HARLOW, ANDREW BESTWICK, EMMANUEL RASHBA, Harvard University, KARSTEN FLENSBERG, University of Copenhagen, CAROLYN STWERTKA, THITI TAYCHATANAPAT, Harvard University, SUSAN WATSON, Harvard University and Middlebury College, CHARLES MARCUS, Harvard University — We use charge sensing of Pauli blockade (including spin and isospin) in a two-electron $^{13}$C nanotube double quantum dot to measure relaxation and dephasing times. The relaxation time, $T_1$, first decreases with parallel magnetic field and then goes through a minimum in a field of 1.4 T. We attribute both results to the spin-orbit-modified electronic spectrum of carbon nanotubes, which suppresses hyperfine mediated relaxation and enhances relaxation due to soft phonons. The inhomogeneous dephasing time, $T_2^*$, is consistent with previous data on hyperfine coupling strength in $^{13}$C nanotubes. This work was supported by the National Science Foundation under grant no. NIRT 0210736 and the GRFP, ARO/iARPA, the Department of Defense, and Harvard’s Center for Nanoscale Systems.

3:18PM L24.00003 Electrical evidence for the encapsulation of $^{14}$C$_{60}$ inside a carbon nanotube: Random telegraph signal and hysteretic current-voltage characteristics
  
1 Supported by the GPP of KICOS and NSI-NCRC of KOSEF, Korea.

3:30PM L24.00004 Breakdown of the Wigner-Mattis theorem in semiconductor carbon-nanotube quantum dots , MASSIMO RONTANI, INFN-CNR Research Center S3, Modena, Italy, ANDREA SECCHI, University of Modena, Italy, FRANCA MANGHI, INFN-CNR S3 and University of Modena, Italy — The Wigner-Mattis theorem states the ground state of two bound electrons, in the absence of the magnetic field, is always a spin-singlet. We predict the opposite result — a triplet — for two electrons in a quantum dot defined in a semiconductor carbon nanotube. The claim is supported by extensive many-body calculations based on the accurate configuration interaction code DONRO-DRIGO (www.s3.infm.it/donrodrigo). The crux of the matter is the peculiar two-valley structure of low-energy states, which encodes a pseudo-spin degree of freedom. The spin polarization of the ground state corresponds to a pseudo-spin singlet, which is selected by the inter-valley short-range Coulomb interaction. Single-electron excitation spectra and STM wave function images may validate this scenario, as shown by our numerical simulations.

3:42PM L24.00005 Casimir Interactions Between Scatterers on Carbon Nanotubes , DINA ZHABIN-SKAYA, University of Pennsylvania, JESSE KINDER, Cornell University, E. J. MELE, University of Pennsylvania — We study the interactions between two short-range scatterers in metallic carbon nanotubes as a Casimir problem. In the massless Dirac Hamiltonian for the electrons, a defect can be represented by a scattering potential with a pseudospin polarization. Sublattice-asymmetric and bond-centered potentials may lead to small momentum backscattering, depending on the chiral angle of the nanotube. Quasibound states formed between two defects determine the forces at the boundaries. We develop a force operator approach within the Dirac model to calculate the forces on two square well potentials of finite width, and take the limit of sharp and strong scatterers to study the Casimir force mediated by the fermions. For the special case of two identical scatterers we recover the conventional one-dimensional attractive Casimir force. For the general problem with inequivalent scatterers we find that the magnitude and sign of this force depends on the relative pseudospin polarizations of the two defect potentials. We will also discuss the effects intervalley scattering on the Casimir interactions between defects.

3:54PM L24.00006 Water confined in carbon nanotubes: Magnetic response and proton chemical shieldings
  
1 Prepared by LLNL under Contract DE-AC52-07NA27344

4:06PM L24.00007 ABSTRACT WITHDRAWN —

4:18PM L24.00008 Effect of spin-orbit interaction on the static polarizability of single-wall carbon nanotubes*, G. S. DINIZ, S. E. ULLOA, Ohio University — The electronic structure of carbon nanotubes (CNTs) is known to exhibit different metallic or insulating behavior as different chiral vectors are considered. Application of external electric fields and the presence of spin-orbit interaction (SOI) result in the Rashba effect modifying the level structure of CNTs, strongly coupling spin and orbital degrees of freedom, as demonstrated in recent experiments [1]. In this work we calculate the static long-wavelength limit of the dielectric response of different single-wall CNTs when subjected to uniform external electric fields both along and across the longitudinal direction (parallel to the nanotube axis). Our calculation uses a π-band tight-binding formalism, considers Rashba and intrinsic SOI, and utilizes the random phase approximation to evaluate $\epsilon(q \rightarrow 0, \omega = 0)$ [2]. We use parameters from the literature and find that the metallic-to-semiconductor transition induced by the intrinsic SOI is suppressed as the Rashba field is taken into account. We further show that this behavior has a clear signature on measurable quantities, such as the static polarizability. We discuss its dependence on nanotube size and chirality and propose possible nanoprobe experiments to study this phenomenon. [1] F. Kuemmeth et al., Nature 452, 448-452 (2008). [2] M. L. Cohen et al., Phys. Rev. B 52, 8541 (1995). *Supported by Fulbright, CAPES and NSF-DMR MWN.
4:30PM L24.00009 Low-Temperature Studies of Electrostatic Doping and Phonon Renormalization in Individual Single-Walled Carbon Nanotubes. GUGANG CHEN, Honda Research Institute USA Inc., Columbus, OH 43212, TEREZA PARONYAN, GAMIH SUMANASEKERA, Department of Physics, University of Louisville, Louisville, KY 40292, ELENA PIGOS, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., Columbus, OH 43212 — Electrostatic doping of carbon nanotubes (CNTs) induced by applied external gate voltage ($V_g$) in the field-effect transistor (FET) configuration allows controllable variation of charge density and the Fermi level in nanotubes. Raman scattering from a CNT is very sensitive to doping and its interaction with the surrounding environment. Recently, the peculiarities of G-mode as a function of gate induced carrier at room temperature have been reported in [1] (Nature Nanotechnology 2, 725 (2007)). In the present work, we used Raman scattering to study the p- and n-electrostatic doping of CNT as a function of $V_g$ in a wide range of temperature from 6.8 K to 300 K. Virtually symmetric blue-shifting of the G-mode for both p- and n-doping of CNTs has been observed. We found that the prehistory of the CNT measurement as well as environment interaction such as gas adsorption on CNT plays an important role on the observed phenomena. Explanation of our findings will be discussed based on phonon energy renormalization of carbon nanotubes [1] due to the carrier density variation during electrostatic doping.

4:42PM L24.00010 Field Enhancement inside Carbon Nanotubes. HONG ZHANG, Sichuan University, China, YOSHISHUKI MIYAMOTO, Nano Electronics Res. Labs., NEC, Japan — There are many investigations on photo-excitations with polarization vector parallel to tube axis (parallel-polarization), compared to it, few studies on those with polarization vector perpendicular to tube axis (cross-polarization) are reported because of early theoretical consideration on electric-field-depolarization effect of nanotubes with cross-polarization [1]. Using dynamical consideration and TDDFT analysis, we herein present the influence of external electric field perpendicular to the axis of semiconductor carbon nanotube (CNT). By adjusting frequency of applied E-field in corresponding wavelength of light from 800nm to 591 nm, the total E-field inside carbon nanotubes has been found to show slow change depending on the frequency; incomplete screening and strong enhancement even without including the excitonic effect [2]. The enhancement comes from increase of oscillating amplitude of electron cloud with resonant frequency given by the applied E-field. Also the numerical stability and the satisfaction of energy conservation rule with application of dynamical E-field were numerically checked [3]. This finding should be taken into account in interpreting a measurement of optical response of molecules being encapsulated in CNTs. [1]. H. Ajiki and T. Ando, Physica B 201, 349 (1994) [2]. S. Uryu and T. Ando, Phys. Rev. B 76, 115420 (2007) [3]. Y. Miyamoto and H. Zhang, Phys. Rev. B 77, 165123 (2008).

4:54PM L24.00011 Quasi-particle Energy Gap of Metal-coated Carbon Nanotubes. YU ZHOU, LI CHEN, YIMING ZHANG, SWASTIK KAR, PULICKEL AJAYAN, SARJU NAYAK, Rensselaer Polytechnic Institute — We have studied the electronic structures of metal-coated carbon nanotubes using density functional theory and many body corrections based on GW approximation (GWA). In particular, we will present energy band gap variation as a function of metal of metal atoms on the nanotube surface. Our results are compared with recent experiments.

5:06PM L24.00012 Microwave Rectification by Carbon Nanotube Schottky Diodes. ENRIQUE COBAS, STEVEN ANLAGE, MICHAEL FUHRER, Department of Physics and Center for Nanophysics and Advanced Materials, University of Maryland College Park — We report the fabrication and electrical characterization of carbon nanotube Schottky diodes (CNT-SDs) via photolithography on high-frequency-compatible substrates using dissimilar contacts of chromium and platinum. The diodes are well-described by the ideal diode equation ($n = 1.0$). DC and low-frequency behavior is compared to a model of a diode in series with a resistor. The diodes rectify microwave signals beyond 18GHz and produce dc currents of hundreds of nanoamperes. The frequency and voltage dependence is used to estimate the junction capacitance of 1aF and an intrinsic device cut-off frequency of 400GHz.


5:18PM L24.00013 Microwave Irradiation Induced Effects to Single-walled Carbon Nanotube Thin Films. LU WANG, University of Arizona, YAO XIONG, Ohio University, ZIRAN WU, University of Arizona, LIWEI CHEN, Ohio University, HAO XIN, University of Arizona — Carbon nanotubes have been considered as potential building blocks for nano-scale circuits in virtue of their unique mechanical and electrical properties. However, one of the biggest obstacles for massive production of nanotube circuits is the difficulty of separating semiconducting tubes from metallic tubes or vice versa. In this work, a convenient method which may be potentially employed to selectively remove metallic tubes using microwave induced breakdown is proposed and investigated. Carbon nanotube thin films deposited on glass and quartz substrates are placed in a commercial microwave oven and heated for up to several minutes. The radial breathing mode in Raman spectra on the nanotube samples before and after the microwave irradiation suggests that the metallic-to-semiconducting ratios are reduced by around 20%. Meanwhile, because in the thin film samples most of the nanotubes are entangled, smaller diameter nanotubes (both metallic and semiconducting) tend to be affected more. THz transmission measurements of these thin films are also performed before and after microwave irradiation. The significant increase of transmission after the microwave irradiation process confirms the loss of metallic tubes.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L25 DMP: Focus Session: Probing and Modifying Materials with Lasers II 327

2:30PM L25.00001 Modeling of Laser Material Interactions. BARBARA GARRISON, Penn State University — Irradiation of a substrate by laser light initiates the complex chemical and physical process of ablation where large amounts of material are removed. Ablation has been successfully used in techniques such as nanolithography and LASIK surgery, however a fundamental understanding of the process is necessary in order to further optimize and develop applications. To accurately describe the ablation phenomenon, a model must take into account the multitude of events which occur when a laser irradiates a target including electronic excitation, bond cleavage, desorption of small molecules, ongoing chemical reactions, propagation of stress waves, and bulk ejection of material. A coarse grained molecular dynamics (MD) protocol with an embedded Monte Carlo (MC) scheme has been developed which effectively addresses each of these events during the simulation. Using the simulation technique, thermal and chemical excitation channels are investigated. The mechanism of ablation for thermal processes is governed by a critical number of bond breaks following the deposition of energy. For the case where an absorbed photon directly causes a bond scission, ablation occurs following the rapid chemical decomposition of material. The study provides insight of stress waves, and bulk ejection of material. A convenient method which may be potentially employed to selectively remove metallic tubes using microwave induced breakdown is proposed and investigated. Carbon nanotube thin films deposited on glass and quartz substrates are placed in a commercial microwave oven and heated for up to several minutes. The radial breathing mode in Raman spectra on the nanotube samples before and after the microwave irradiation suggests that the metallic-to-semiconducting ratios are reduced by around 20%. Meanwhile, because in the thin film samples most of the nanotubes are entangled, smaller diameter nanotubes (both metallic and semiconducting) tend to be affected more. THz transmission measurements of these thin films are also performed before and after microwave irradiation. The significant increase of transmission after the microwave irradiation process confirms the loss of metallic tubes.

3:06PM L25.00002 Molecular dynamics simulation study of the ejection and transport of polymer molecules in matrix-assisted pulsed laser evaporation. LEONID ZHIGILEI, ELODIE LEVEUGLE, University of Virginia — There are a number of applications that utilize the ability of laser ablation of a volatile matrix to entrain, eject and, if needed, deposit large macromolecules to a substrate with minimum chemical modification. In particular, the Matrix-Assisted Pulsed Laser Evaporation (MAPLE) technique is used in fabrication of ultra-thin organic films for optoelectronic, biomedical, and chemical sensor applications. In this presentation we report the results of a computational investigation of the mechanisms of molecule ejection in MAPLE. Coarse-grained molecular dynamics simulations are performed for polymer concentrations up to 6 wt.%. Contrary to the original picture of the ejection and transport of individual polymer molecules in MAPLE, the simulations indicate that polymer molecules are only ejected as parts of polymer-matrix clusters/droplets generated in the process of the explosive disintegration of the overheated matrix. An internal release of matrix vapor in the overheated droplets is shown to be capable of pushing polymer molecules to the outskirts of the droplets, forming “molecular balloons” in which polymer-rich surface layers enclose the volatile matrix material. The results of the simulations explain some of the complex morphologies observed in polymer films deposited in MAPLE and conventional polymer ablation/deposition experiments.

4:30PM L24.00009 Low-Temperature Studies of Electrostatic Doping and Phonon Renormalization in Individual Single-Walled Carbon Nanotubes. GUGANG CHEN, Honda Research Institute USA Inc., Columbus, OH 43212, TEREZA PARONYAN, GAMIH SUMANASEKERA, Department of Physics, University of Louisville, Louisville, KY 40292, ELENA PIGOS, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., Columbus, OH 43212 — Electrostatic doping of carbon nanotubes (CNTs) induced by applied external gate voltage ($V_g$) in the field-effect transistor (FET) configuration allows controllable variation of charge density and the Fermi level in nanotubes. Raman scattering from a CNT is very sensitive to doping and its interaction with the surrounding environment. Recently, the peculiarities of G-mode as a function of gate induced carrier at room temperature have been reported in [1] (Nature Nanotechnology 2, 725 (2007)). In the present work, we used Raman scattering to study the p- and n-electrostatic doping of CNT as a function of $V_g$ in a wide range of temperature from 6.8 K to 300 K. Virtually symmetric blue-shifting of the G-mode for both p- and n-doping of CNTs has been observed. We found that the prehistory of the CNT measurement as well as environment interaction such as gas adsorption on CNT plays an important role on the observed phenomena. Explanation of our findings will be discussed based on phonon energy renormalization of carbon nanotubes [1] due to the carrier density variation during electrostatic doping.
3:18PM L25.00003 Mechanism of Resonant Mid-Infrared Laser Ablation of Polystyrene, RICHARD HAGLUND, Vanderbilt University, STEPHEN JOHNSON, University of Kentucky, DANIEL BUBB, Rutgers University—Camden — We investigated the mechanism of resonant-infrared laser ablation of polymers using polystyrene as a model material. The ablation laser was a picosecond mid-infrared free-electron laser tuned to mid-IR laser wavelengths that are resonant with specific vibrational modes of the polystyrene target. Time-resolved plume imaging combined with etch-depth measurements and finite-element calculations indicate that a blowoff model fits the experimentally measured etch depths and plume images, provided one accounts for moderate shielding of the surface by the ablation plume. The finite-element model includes the temperature-dependent absorption coefficient and specific heat that dramatically change the material properties above the glass-transition temperature. Ablation begins after a thin surface layer of the material is superheated to temperatures exceeding 1000 C and undergoes spinodal decomposition. The majority of the ablated material is then expelled by way of recoil-induced ejection as the pressure of the expanding vapor plume compresses a laser-melted area at the target surface.

3:30PM L25.00004 The influence of thermal confinement and temperature-dependent absorption on resonant infrared ablation of frozen aqueous and alcohol targets, DANIEL BUBB, STEPHEN JOHNSON, RICHARD HAGLUND, Vanderbilt — We investigated the mechanism of matrix-assisted resonant infrared laser ablation in frozen aqueous and methanol solutions of polymer, by performing plume shadowgraphy and ablation yield measurements. A picosecond, tunable free-electron laser was used for ablation at two wavelengths, one (2960 nm) that was resonant with the –OH stretch in both water and methanol, and the other (3450 nm) that is resonant with the –CH stretch in methanol. The plume images showed gross similarities, differing only in the time required for the shockwave to appear and in the velocity of the shock front. Typically, 15-25 µs after the ablation laser pulse arrives the primary material ejection commences and lasts for hundreds of µs. In all three cases, the ablation plume appears to consist entirely of vapor with no droplets or solid particles. The ablation yield is either linear or quadratic in fluence. This dependence can be understood if we consider thermal diffusion in the targets and the temperature dependence of the absorption coefficient.

3:42PM L25.00005 VUV excimer laser-materials interactions with fluorocarbon polymers, TOM DICKINSON, SHARON GEORGE, STEVE LANGFORD, Washington State University — Particle emission from transparent wide bandgap materials at laser fluences below the threshold for optical breakdown can provide important insight on interactions at the higher fluences employed for surface modification, machining, and laser ablation deposition. We present recent studies of ion and neutral molecule emission from polytetrafluoroethylene [(C₂F₅)ₙ—PTFE—Teflon®] and polyvinylidene fluoride [(CH₂CF₂)n—PVDF] during nanosecond pulsed 157-nm excimer laser irradiation. The chemical and electrical properties of these materials play important roles in many technologies. In PTFE, the primary mechanism for material removal involves bond scission along the backbone of the polymer. In PVDF, HF emission is accompanied by carbonization of the irradiated region. High-energy positive and negative ions are observed from both materials under 157-nm irradiation. We describe critical measurements that reveal the physics and chemistry underlying these processes.

4:06PM L25.00007 Laser Interactions with Vertically-Aligned Carbon Nanotube Arrays, DAVID GEOHEGAN, Oak Ridge National Laboratory, CHRIS ROULEAU, ALEX PURETZKY, JEREMY JACKSON, NORBERT THONNARD, ILIA IVANOV, KARREN MORE, CNMS AND MSTD, OAK RIDGE NATIONAL LABORATORY TEAM — Femtosecond and nanosecond laser interactions with vertically aligned carbon nanotube arrays (VANTA)s have been studied in vacuum and background gases. As-grown VANTAks were synthesized by chemical vapor deposition onto Fe/Al-coated Si wafers to typical heights of 10-20 microns. The forests of aligned nanotubes grow from catalyst nanoparticles anchored to the substrate and typically have a disordered layer of nanotubes at their top surfaces. Laser interactions in vacuum, inert, and oxidizing atmospheres were compared. The nanotubes were found to form periodic surface structures in response to repeated laser pulses. Patterning of the nanotube arrays with scanning beams was studied. Damage to the nanotubes was studied by Raman spectroscopy and high-resolution TEM.

4:18PM L25.00008 Temperature-dependent energy-transfer between electrons and phonons in nickel around Curie temperature and its relation to ultra-fast demagnetization, XUAN WANG, Florida State University, SHOUHUA NIE, Carnegie Mellon University, JUNJIE LI, RICK CLINITE, JIM CAO, Florida State University, JIM CAO TEAM — We report on the use of Ultrafast Electron Diffraction (UED) to study the ultrafast dynamics of nickel induced by fs-laser excitation. Particularly, we have observed a significant increase of electron-phonon coupling time when the pre-set sample base-temperature is reduced across its Curie temperature. This implies a strong quenching of magnetic ordering (ultrafast demagnetization), which serves as an extra energy reservoir other than lattice to relax the electron energy. By modeling the energy transfer among these three systems, we conclude that ultrafast demagnetization happens in a time-scale even shorter than electron-phonon coupling and one temperature for both electron and magnetic ordering, as suggested by several former studies, works very well from energy point of view. Our results also support the former observed ultrafast demagnetization in itinerant ferromagnets, which happens in sub-ps time scale.

1 Research supported by AppliFlex LLC through an NSF-STTR grant.
2 Research supported by a Cottrell College Award from Research Corporation and Awards DMI-0613837 and CMMI-0727713 from the National Science Foundation
3 Research sponsored by DOE-BES (DSUF) at the Center for Nanophase Materials Sciences and ShaRe Facilities.
4:30PM L25.00009 Ultrafast Time Resolved Reflection High-Energy Electron Diffraction Study of Laser-Matter Interactions for Silicon. The work is supported by DOE BES and Materials Research Laboratory.

4:42PM L25.00010 Ultrafast Photoinduced Structural Dynamics in Graphite. This work was supported by the Robert A. Welch Foundation.

5:06PM L25.00012 Photo-irradiation effect on charge-ordered states in strongly correlated electron systems. The work is supported by DOE BES and Materials Research Laboratory.

5:18PM L25.00013 Optical, Mechanical, and Opto-Mechanical Switching of Anchored Dithioazobenzene Bridges. The project is supported by the Robert A. Welch Foundation.

Tuesday, March 17, 2009 2:30PM - 5:30PM Session L26 DMP: Focus Sessions: Graphene VI: Phonons and Raman Spectroscopy 328

2:30PM L26.00001 Photovoltaic Hall Effect in Dirac systems – Application to Graphene. This work was supported by the Robert A. Welch Foundation.

2:42PM L26.00002 Thermal conductivity and thermal rectification in graphene nanoribbons: a molecular dynamics study. The project is supported by the Robert A. Welch Foundation.
2:54PM L26.00003 Raman scattering in bilayer graphene: probing phonons, electrons and electron-phonon interactions. LEANDRO M. MALARD, Departamento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil — The application of resonance Raman spectroscopy to study the electronic, vibrational and electron-phonon interaction properties in bilayer graphene will be presented. From the dependence of the second-order Raman bands on the laser excitation energy, we obtain experimental values for the Slonczewski-Weiss-McClure band parameters of bilayer graphene. We will discuss in detail the effect of each one of the tight band parameters on the electronic structure, showing that bilayer graphene has a larger electronic-phonon asymmetry compared to graphene. We will also present experimental results for the phonon dispersion relations near the K point, showing a strong Kohn anomaly for one of the phonon branches. In a gating experiment, the change in Fermi level of bilayer graphene gives rise to a symmetry breaking, allowing the observation of both the symmetric (S) and anti-symmetric (AS) phonon modes. The dependence of the energy and damping of these phonon modes on the Fermi level energy is explained in terms of distinct couplings of the S and AS phonons with intra- and inter-band electron-hole transitions.

3:30PM L26.00004 Phonon dispersion of graphene revisited. SILVIA VIOLA KUSMINSKY, DAVID CAMPBELL, ANTONIO CASTRO NETO, Boston University — We calculate the phonon spectrum for a graphene sheet resulting from the model proposed by T. Lenosky et al. (Nature 355, 333 (1992)) for the free energy of the lattice. This model takes into account not only the usual bond bending and stretching terms, but captures the possible misalignments of the p₆ orbitals. We compare our results with previous models used in the literature. We analyze the effect of anharmonic terms.

3:42PM L26.00005 Giant nonadiabatic effects in layer metals: Raman spectra of intercalated graphite and doped graphene explained. A. MARCO SAITTA, MICHELE LAZZERI, MATTEO CALANDRA, FRANCESCO MAURI, IMPMC, Paris, France — The occurrence of nonadiabatic effects in the vibrational properties of metals has been predicted since the 1960s [1], but hardly confirmed experimentally. We report the first fully ab initio calculations of nonadiabatic frequencies of a number of conventional (hcp Ti and Mg), layered metals (MgB₂, CaC₆, other intercalated graphites) [2] and doped graphene [3]. Nonadiabatic effects can be spectacularly large (up to 30% of the phonon frequencies), but they can only be experimentally observed in the Raman spectra of layered compounds. In layered metals nonadiabatic effects are crucial to explaining the observed Raman shifts and linewidths. Moreover, we show that those quantities can be used to extract the electron momentum-relaxation time. [1] S. Engelsberg and J.R. Schrieffer, Phys. Rev. 131, 993 (1962). [2] A.M. Saitta et al., Phys. Rev. Lett. 100, 226401 (2008). [3] M. Lazzeri and F. Mauri, Phys. Rev. Lett. 97 , 266407 (2006).

3:54PM L26.00006 Probing the Intrinsic Properties of Exfoliated Graphene: Raman Spectroscopy of Free-Standing Monolayers. STEPHANE BERCAUD, SUNMIN RYU, LOUIS BRUS, TONY HEINZ, Columbia University — The properties of pristine, free-standing graphene monolayers prepared by mechanical exfoliation of graphite are investigated. The graphene monolayers, which were suspended over open trenches, are examined by means of spatially resolved Raman spectroscopy of the G, D, and 2D phonon modes. The G-mode phonons exhibit low energies (1580 cm⁻¹) and broad widths (14 cm⁻¹) compared to the response for samples supported on the SiO₂-covered substrate. From analysis of the G-mode Raman spectra, we deduce that the free-standing graphene monolayers are essentially undoped, with an upper bound of 2×10¹⁴ cm⁻² for the residual carrier concentration. On the supported regions, significantly higher and spatially inhomogeneous doping is observed. The free-standing graphene monolayers show very little local disorder, based on the very low Raman D mode intensity.

4:06PM L26.00007 Micro Raman spectroscopy of graphene Hall Bars in the QHE regime. SEBASTIAN REMI, CONSTANZE METZGER, ANNA SWAN, BENNETT B. GOLDBERG, Boston University — One of the most intriguing aspects in the physics of graphene are new types of quantum Hall effects which differ significantly from observations on conventional 2DEG samples. Furthermore the Raman spectrum of graphene shows charge carrier dependent Kohn anomalies. So far transport and optical measurements on graphene haven’t been combined to explore the behavior of the Raman features dependent on the Landau levels. We present our latest measurements of Raman scattering on graphene single and bilayers in the Quantum Hall regime.

4:18PM L26.00008 ABSTRACT WITHDRAWN —

4:30PM L26.00009 Raman Scattering from Pt Island-Decorated Graphene. AWNISH GUPTA, HUMBERTO GUTIERREZ, Department of Physics, Pennsylvania State University, PETER EKLUND, Department of Physics, Department of Material Science and Engineering, Pennsylvania State University — We performed microRaman studies of decorated n–Graphene Layers (nGLs). Nano-islands (NI; dia~5-10 nm) of Pt were created by deposition on the nGL with gaps between the NI in the range of few nm. When the NI were present, we observed D and D’ Raman bands as well as splitting of the G-band into G⁺ and G⁻ (most pronounced for 1GL). The observations may be related to graphene “confined” in the interstitial spaces between NIs. The D and D’ bands show the following properties: (1) Intensity of D and D’ relative to G band decreases with increasing number of layers n between the nGL. (2) Peak frequencies, ωD increases linearly with 1/n while ωD’ remains constant. (3) Linewidth ΓD decreases linearly with 1/n, while ΓD’ increases linearly with 1/n. Our results will be discussed in terms of results theoretically predicted by zone folding (Jishi et al).

1This work was supported by the NSF NIRT ECS0609243

4:42PM L26.00010 Raman Spectroscopy of the 2D Mode in Free-Standing Graphene Multilayers. JANINA MAULTZSCH, T.U. Berlin, Germany, STEPHANE BERCAUD, LOUIS BRUS, TONY HEINZ, Columbia U., New York, NY 10027 — Raman spectroscopy of the 2D (or G') mode is a critical tool for the analysis of graphene mono- and multilayers. This symmetry-allowed overtone mode permits one to probe zone-edge phonons by Raman spectroscopy. Moreover, its doubly-resonant electronic character renders it readily observable and encodes in it information about the electronic structure of the graphene sample. In particular, the 2D mode provides a clear signature of the thickness of mono- and multilayer graphene films. In this paper, we present a detailed study of the properties of the 2D for a pristine, free-standing graphene monolayer prepared by mechanical exfoliation over a trench structure. In contrast to the behavior of monolayers of graphene on substrates, for this pristine graphene sample, we observe a positively skewed line shape. The linewidth is also somewhat reduced compared to that observed for graphene supported on a substrate. Further, the 2D mode in the free-standing graphene films exhibits a slightly stronger dispersion with energy of the pump photons than for supported monolayers. We discuss our findings within the framework of double resonance theory, taking into account the intrinsically undoped nature of the free-standing graphene samples. J. Maultzsch et al., Phys. Rev. B 70, 155403 (2004) A. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006)
4:54PM L26.00011 Seeing and counting graphene layers by elastic light scattering, C. CASIRAGHI, Cambridge University, UK, A. HARTSCHUH, LMU Munich, Germany, E. LIDORIKIS, Ioannina University, Greece, H. QIAN, H. HARUTYUNYAN, T. GOKUS, LMU Munich, Germany, K. S. NOVOSELOV, Manchester University, UK, A. C. FERRARI, Cambridge University, UK — Raman scattering has recently emerged as a viable and nondestructive technique for the identification of graphene, its doping, edges and amount of defects [1-3]. However, the Raman scattered photons are a minority compared to those elastically scattered. Here we show that large graphene layers can be mapped and identified in a few minutes by elastic scattering. We report an extensive investigation of graphene on silicon/silicon oxide substrate by monochromatic and white-light elastic scattering and the theoretical understanding of the experimental data [4]. Maps of the scattered light are obtained by raster scanning the sample with a piezo-electric stage. We show that the image contrast depends sensitively on the dielectric properties of the sample as well as the substrate geometry and can be described quantitatively using the complex refractive index of bulk graphite. [1] A. C. Ferrari et al., PRL 97, 187401 (2006) [2] S. Pisana et al., Nature Materials 6, 198 (2007) [3] C. Casiraghi et al., APL 91, 233108 (2007) [4] C. Casiraghi et al., Nano Letters 7, 2711 (2007)

5:06PM L26.00012 Polarized micro Raman spectroscopy of bilayer graphene, HYERIM MOON, DUHEE YOON, Department of Physics, Sogang University, Seoul 121-742, Korea, YOUNG-WOO SON, Korea Institute for Advanced Study, Seoul 130-722, Korea, HYEONSIK CHEONG, Department of Physics, Sogang University, Seoul 121-742, Korea — The frequency of Raman 2D band of the graphite depends on the excitation laser energy. This phenomenon is explained with double resonance Raman process. In polarized micro-Raman spectroscopy of single layer graphene, Raman G band (∼1586 cm⁻¹) is isotropic, and 2D band (∼2686 cm⁻¹) strongly depends on relative polarizations of the incident and scattered photons. This strong polarization dependence originates from inhomogeneous optical absorption and emission mediated by resonant electron-phonon interaction. In bi-layer graphene, Raman 2D band can be decomposed into four Lorentzian peaks which can be interpreted in terms of the four transition paths in the double resonance Raman process. We investigated the polarization dependence of each Lorentzian peak in the Raman 2D band of bi-layer graphene for different excitation laser energies. Strong polarization dependence of the polarized Raman scattering is analyzed in terms of the band structure of bi-layer graphene.

Tuesday, March 17, 2009 2:30PM - 4:42PM
Session L27 FLAP: Focus Session: Graphene Device and Applications II

2:30PM L27.00001 Graphene and chemically modified graphene sensors, JEREMY ROBINSON, Naval Research Laboratory — Molecular sensing via sp²-bonded carbon nanomaterials is a promising research area in both nanoscience and nanotechnology. In general these materials are thermally and chemically stable, come in a variety of different geometries (spheres, tubes, and sheets), and are process compatible with conventional micro-lithographic techniques. In this talk we focus on atomically thin sheets of sp²-bonded carbon, known as graphene, and discuss their sensing properties when exposed to chemical vapors. The remarkable physical properties of graphene—from near ballistic electron conduction to ultra high stiffness (≈5 times that of steel)—make it a unique system to study both electronic and mechanical transduction modes. Finally, we demonstrate the utility of graphene-based films is greatly expanded after chemical functionalization. In this regard, chemically modified graphene (CMG) is emerging as a material system whose properties are complementary to nominally pure graphene for sensing applications.

3:06PM L27.00002 Intrinsic Response of Graphene Vapor Sensors, YE LU, YAPING DAN, University of Pennsylvania, NICHOLAS KYBERT, University of Warwick, CHARLIE JOHNSON, University of Pennsylvania — Ye Lu, Yaping Dan, Nicholas J. Kybert, A. T. Charlie Johnson, 1 University of Pennsylvania, USA 2 University of Warwick, UK Graphene is a purely two-dimensional material that has extremely favorable chemical sensor properties. It is known, however, that conventional nanolithographic processing typically leaves a resist residue on the graphene surface, whose impact on the sensor characteristics of the system has not yet been determined. Here we show that the contamination layer both degrades the electronic properties of the graphene and masks graphene’s intrinsic sensor responses. The contamination layer chemically dopes the graphene, enhances carrier scattering, and acts as an absorbent layer that concentrates analyte molecules at the graphene surface, thereby enhancing the sensor response. We demonstrate a cleaning process that verifies the contamination on the device structure and allows the intrinsic chemical responses of graphene to be measured. Additionally, methods of functionalizing clean graphene device as high quality chemical vapor sensor are explored. Funding: JSTO DTRA and the Army Research Office Grant #W911NF-06-1-0462, NSF-NSEC/N Birck DMR-0425780, REU program of the Laboratory for Research on the Structure of Matter (N.I.K.).

3:18PM L27.00003 Single-layer graphene Motion and Mass Sensors with Electrical Readout, CHANGYAO CHEN, Columbia University, SAMI ROSENBLATT, KIRILL BOLOTIN, HORST STORMER, PHILIP KIM, TONY HEINZ, JAMES HONE — We report for the first time the implementation of graphene electromechanical resonators that can detect their own motion. Susspeed single-layer graphene field-effect transistors allow for electrical detection of the resonances while functioning as heterodyne mixers in a manner analogous to the operation of a radio receiver. Mechanical resonances occur in the 10-100 MHz range, can be lithographically-tailored, are tunable by tens of MHz, and have quality factors up to 200 while operated in vacuum at room temperature. Furthermore, by analyzing the frequency response of the resonators, we succeed in weighing both the pristine single-layer graphene and with a layer of organic material deposited on.
3:30PM L27.00004 Electronic and magnetic functions of nanographene-based host-guest system. TOSHIKAZU ENOKI, Tokyo Institute of Technology — The electronic structure of nanographene having open edges crucially depends on its edge shape. According to theoretical predictions, nanographene has nonbonding =-electron state (edge state) localized in zigzag edges. We investigated the electronic structure of graphene edges, the magnetism of the edge-state spins in nanographene and the effect of host-guest interaction on the magnetism. For magnetic investigations, we employed nanoporous activated carbon fiber (ACF) having a 3D disordered network of nanographite domains, each of which is a stack of 3-4 nanographene sheets. STM/STS investigations of hydrogen-terminated graphene edges confirm the presence of edge states around zigzag edges, in good agreement with theoretical works. The feature of the edge state depends on the detailed geometry of the edge structures. The magnetism of nanographene in ACF has a ferrimagnetic feature with a net magnetic moment, for which the cooperation of ferromagnetic intra-zigzag-edge and ferromagnetic/antiferromagnetic inter-zigzag-edge interactions is responsible. Heat-treatment, which induces an insulator-metal transition, brings about spin glass state of the edge-state spins in the vicinity of the transition. Physorption of guest species such as water, organic molecules, rare gas in the ACF nanopores generates a high-spin/low-spin magnetic switching phenomenon, in which a discontinuous reduction of the magnetic moment takes place. This is explained in terms of the strengthening of the inter-graphene-sheet antiferromagnetic interaction, which is induced by the mechanical compression of nanographite domains by the condensed guest molecules. The magnetic oxygen molecules physisorbed in the nanopores work seriously to decrease the magnetoresistance in ACF as a consequence of the interaction between the oxygen molecule spins and edge-state spins.

4:06PM L27.00005 Investigation of Molecular Functionalizing Agents for Graphene Device Optimization. DAMON FARMER, IBM, YU-MING LIN, ALI AFZALI-ARDAKANI, PHAEDON AVOURIS — Due to its linear dispersion relation and the predicted chiral nature of its quasiparticles, graphene has become a material of intense experimental and theoretical investigation. There has been rapid progress in the fabrication and understanding of graphene devices. However, many key issues still need to be addressed in order to fully exploit graphene for technological applications. Here, we identify stable molecular compounds that can be used as dopants and functionalizing agents on graphene. As dopants, these compounds are used to both modify the potential profile in the channel region of graphene devices, and reduce parasitic resistances in these devices. As functionalizing agents, these compounds serve as nucleation sites for the uniform growth of thin high-κ gate dielectrics, allowing for enhanced capacitive coupling with the graphene channel. The characteristics of graphene devices employing these molecular compounds will be presented, and problems associated with the implementation of these molecules in graphene devices will be discussed.

4:18PM L27.00006 Fabrication and Chemical Doping of Carbon-based Transparent Electrodes. GEORGE TULEVSKI, IBM T.J. Watson Research Center, ALI AFZALI — The use of carbon-based materials (carbon nanotubes and graphene) as transparent electrodes has attracted enormous interest due to their high transparencies, conductivity and potential as a lower cost alternative to traditional transparent electrode materials (i.e. Indium Tin Oxide). This talk will focus on using solution processes to suspend both carbon nanotubes and graphene flakes in solution and the fabrication of transparent electrodes from these solutions. Solutions were prepared using both surfactants and organic solvents, followed by purification to remove large aggregates and impurities. A variety of chemical dopants were then employed including metal salts and small organic molecules. The sheet resistance of the resultant films can be significantly reduced with chemical doping.

4:30PM L27.00007 Atomic Layer Deposition (ALD) methods for fabricating graphene devices - theory and experiments. Yvette Hancock, Department of Engineering Physics, Helsinki University of Technology, Finland, Saimiul Haque, Nokia Research Center, Helsinki, Finland, Maarit Karppinen, Laboratory of Inorganic Chemistry, Department of Chemistry, Helsinki University of Technology, Finland, Nasa Staralouet, Department of Physics, Helsinki University of Technology, Finland — ALD has the potential to be a well controlled method for coating and patterning graphene structures and making new generation devices. We have investigated the ALD of 5 nm thin coatings of high-κ dielectric Al2O3 onto graphene, and have determined the selectivity of the chemical specific deposition, for example, to the edges or starting from defect sites. Experimentally, we see an affinity for Al2O3 to coat the edges of graphene, which is also supported by our ab initio calculations. The affinity of the Al2O3 coating with the edges of graphene allows us to make a mask, which could then be used to fabricate graphene nanoribbons of widths less than 50 nm that are also gated.

Tuesday, March 17, 2009 2:30PM - 5:18PM —
Session L28 DMP FLAP: Focus Session: Thermoelectric Materials: Tellurides 330

2:30PM L28.00001 Enhancement of the thermoelectric figure of merit by distortions of the dispersion relation. Joseph P. Heremans, Department of Mechanical Engineering and Department of Physics, The Ohio State University — A doubling of the thermoelectric figure of merit (ZT) of p-type PbTe above 700 K has been recently demonstrated (1) in thallium-doped material. The effect comes about because of an electronic energy level of the Tl atoms resonates with the valence band of PbTe. This creates an excess density of states, g(E), at a specific energy about 60 meV below the valence band edge, which in turn gives a thermoelectric power at that carrier concentration about three times higher than that of similarly-doped p-type PbTe. In this talk, we will review the mechanisms by which this distortion of the g(E) function, from the normal E1/2 form valid for parabolic bands in three dimensions into a spike-like function, increases the thermoelectric power and thus ZT. We further derive a set of criteria for the excess g(E) to improve ZT. We will discuss the applicability of this approach to other electronic levels in PbTe first, and then describe the more general quest for such energy levels in other thermoelectric semiconductors. (1) J. P. Heremans et al., Science 321 554 (2008)

3:06PM L28.00002 Electronic Inhomogeneity in PbTe-based High Performance Thermoelectric Materials Observed by NMR. E.M. Levin, K. Schmidt-Rohr, B.A. Cook, Ames Laboratory DOE and Iowa State University, M.G. Kanatzidis, Northwestern University — Effects of composition and synthesis conditions on the local structure and charge carrier concentration in AgxSb2Pb1−xTe20 (LAST-18) thermoelectric (TE) materials have been studied by 125Te and 207Pb nuclear magnetic resonance (NMR) with magic-angel spinning. The high-resolution 125Te NMR spectra show that most Sb and Ag is not part of Sb2Te3, AgSbTe2, or Ag2Te inclusions. Biexponential NMR spin-lattice (T1) relaxation as well as Knight shifts of 125Te and 207Pb NMR signals show that many LAST-18 materials contain two phases of similar composition but with free electron concentrations that differ by more than an order of magnitude, i.e. these materials are electronically inhomogeneous. The NMR data were calibrated against Hall- and Seebeck-effect measurements to give the charge carrier concentrations in the two phases. This electronic inhomogeneity may result from the appearance of potential barriers inside TE materials, similar to those observed for semiconductor-semiconductor or metal-semiconductor junctions. Such barriers may affect thermopower, electrical, and thermal conductivity of TE materials.
3:18PM L28.00003 Thermodynamic Properties of Pb and Ag-Sb Based Chalcogenides: A First-Principles Study1, Yi ZHANG, University of Nevada, Las Vegas, XUEZHI KE, University of Nevada Las Vegas; East China Normal University, CHANGFENG CHEN, University of Nevada, Las Vegas, JIHUI YANG, General Motors, PAUL R. C. KENT, Oak Ridge National Lab — The Pb and Ag-Sb based chalcogenide compounds have received considerable interest for their potential applications in thermoelectric devices. Their low thermal conductivity plays a key role in producing the high figure of merit (ZT) that is critical for applications. We performed a series of first-principles calculations on several Pb and Ag-Sb based chalcogenide compounds to understand their lattice dynamics. The direct force method and density functional theory calculations were used to obtain the phonon dispersion and density of states. The phonon softening processes with the volume change were carefully evaluated. Moreover, we employed the quasiharmonic approximation to calculate the thermodynamic functions. The calculated results are in good agreement with available experimental data and provide insights for understanding the physical properties.

1Work supported by DOE grants DE-FG52-06NA20274, DE-FG-0604NT42278, DE-AC02-98CH10886. This research used resources of the National Center for Computational Sciences and the Center for Nanophase Materials Sciences at ORNL.

3:30PM L28.00004 Link between changes in ZT and microstructure in AgSbTe2. PETER SHARMA, JOSHUA SUGAR, DOUGLAS MEDLIN, Sandia National Laboratory — The best thermoelectric alloys have complex microstructures. For example, the LAST alloys, (AgSbTe2)x−y(PbTe)y, possess ZT~1.5–2 but have a great variety of inclusions with different chemistry at different length scales. How does microstructure affect thermoelectric efficiency? Since the phase diagram of this and most quaternary alloys is poorly known, transport properties have not been systematically connected to microstructure. We are attacking this problem by studying the simple ternary alloy AgSbTe2, a component of the LAST system, in order to show how thermoelectric properties change with a known, controlled microstructure. AgSbTe2 forms within the well-studied Ag2Te-Sb2Te3 pseudobinary phase diagam. We have found that Sb-rich AgSbTe2 is composed of Sb2Te5 precipitates embedded in a homogeneous rocksalt Ag10Sb30Te54 matrix. The precipitates are plate-like and crystallographically aligned along their close packed planes parallel to that of the matrix. The size of these Sb2Te5 plates can be tuned from the nanometer to micron scale. In this work, the formation and growth of precipitates over a wide length scale is linked to changes in thermoelectric properties for the first time. This study is useful for understanding the complexity of LAST, or any bulk thermoelectric where second phase precipitation occurs.

3:42PM L28.00005 Microstructure and Nucleation Mechanism for Nanoprecipitates in PbTe-Ag5Sb2Te2. XUEZHI KE, University of Nevada, Las Vegas; East China Normal University, CHANGFENG CHEN, University of Nevada, Las Vegas, JIHUI YANG, General Motors, LIJUN WU, JUAN ZHOU, QIAN LI, YIMEI ZHU, Brookhaven National Laboratory, PAUL R.C. KENT, Oak Ridge National Laboratory — Many recent advances in thermoelectric (TE) materials are attributed to their nanoscale constituents. Determination of the nanocomposite structures has represented a major experimental and theoretical challenge and eluded previous attempts. Here we present the first atomically resolved structures of high performance TE material PbTe-Ag5Sb2Te2 by transmission electron microscopy imaging and density functional theory calculations. The results establish an accurate structural characterization for PbTe-Ag5Sb2Te2 and identify the interplay of electric dipolar interactions and strain fields as the driving mechanism for nanoprecipitate nucleation and growth, which provides key insights for understanding a broad class of complex nanocomposite materials.

3:54PM L28.00006 Galvanomagnetic and Thermomagnetic Properties of Ag1−xNaSb2Te5 Alloys. MICHELE NIELSEN, VLADIMIR JOVOVIC, CHRISTOPHER JAWORSKI, Department of Mechanical Engineering, Ohio State University, Columbus, OH, JOSEPH HEREMANS, Department of Mechanical Engineering and Department of Physics, Ohio State University, Columbus, OH — Group I-V-VI alloys have intrinsically low thermal conductivity1 on the order of 0.65 W/mK due to Umklapp phonon-phonon scattering. Combined with the high valence band density of states in AbSb2Te3, this makes this material system ideal for thermoelectric applications up to 416 K, where AgSbTe2 undergoes a crystallographic phase transition. The partial substitution of Na for Ag is expected to address this problem. We synthesize bulk Ag1−xNaSb2Te5 alloys and measure the evolution of the phase transition as a function of Na concentration x. The thermoelectric and galvanomagnetic properties of the alloys are also studied; based on the measurement of resistivity, Seebeck, Nernst and Hall coefficients we calculate mobilities, Fermi energies and partial carrier concentrations of holes and electrons.

4:06PM L28.00007 Electronic and Thermal Properties of Cubic Ge-Sb-Te Compounds. DONALD MORELLI, KEVIN ZHOU, Michigan State University — The ternary rocksalt structure compound Ge4SbTe5 is unusual because most members of the Ge-Sb-Te family form along the tie-line of the binary compounds GeTe and Sb2Te3, and thus do not possess the 1:1 cation:anion ratio necessary to present themselves in a cubic structure. The TE properties of these (GeTe)2(Sb2Te3)x−y compounds, while interesting in their own right, are no better than those of commercially available materials. To understand the thermoelectric properties of these materials, we investigated the structural and thermal properties of the AlTe3 and Al2Te5 compounds and associated with TE properties a cubic compound is advantageous because there is no issue regarding anisotropy of the thermoelectric properties. We have fabricated bulk samples of Ge4SbTe5 and related compounds, characterized their crystal structure, and measured some of their thermal and electronic properties. Results of isoelectronic substitution of Se on the Te site and Sn on the Ge site will be reported.

4:18PM L28.00008 Thermoelectric Figure-of-merit in Bulk p-type PbTe. BO YU, HUI WANG, Boston College, BED POUMEL, GMZ Energy Inc., KENNETH MCENANEY, GANG CHEN, Mass. Institute of Technology, ZHIFENG REN, Boston College, BOSTON COLLEGE, DEPT. OF PHYSICS TEAM, MASS. INSTITUTE OF TECHNOLOGY, DEPT. OF MECHANICAL ENGINEERING COLLABORATION — Lead telluride and its relatives, with equal numbers of atoms on the cation and anion sites, form stably in the cubic rocksalt structure. For compounds, while interesting in their own right, are no better than those of commercially available materials. To understand the thermoelectric properties of these materials, we investigated the structural and thermal properties of the AlTe3 and Al2Te5 compounds and associated with TE properties a cubic compound is advantageous because there is no issue regarding anisotropy of the thermoelectric properties. We have fabricated bulk samples of Ge4SbTe5 and related compounds, characterized their crystal structure, and measured some of their thermal and electronic properties. Results of isoelectronic substitution of Se on the Te site and Sn on the Ge site will be reported.

4:30PM L28.00009 Modular assembly of binary nanocrystal composite solids for high-efficiency thermoelectric power generation. DONG-KYUN KO, University of Pennsylvania, Materials Sci. & Eng., CHRISTOPHER MURRAY, University of Pennsylvania, Materials Sci. & Eng. and Chemistry — Despite the numerous advantages of semiconductor nanostructures, doping nanometer size crystals show difficulties not found in conventional bulk systems. Especially for thermoelectric applications, it is critical to control the number of carriers that are available in semiconductors in order to maximize the figure of merit. Here, we report modular assembly of binary composite nanocrystals, as an effective bottom-up design tool, to create a new family of artificial solids with a prescribed set of doping levels. Silver telluride (Ag2Te) nanocrystals, which can act as dopants, are introduced in lead telluride (PbTe) nanocrystal assemblies in order to modify the carrier concentration until an optimum power factor is realized. This study focuses on electronic and thermoelectric characterization of these binary composite solids. Hall measurement and field effect transistor characteristics were investigated in order to identify the carrier type, mobility, and concentration. Temperature dependence of low-bias conductivity was also characterized to gain a better understanding of electronic conduction. Finally, Seebeck voltage was measured with varying PbTe to Ag2Te nanocrystal concentration ratios in order to investigate the Seebeck coefficient as a function of carrier concentration.
4:42PM L28.00010 Galvanomagnetic and thermomagnetic properties of thallium doped Pb-SnTe and PbSeTe1, VLADIMIR JOVOVIC, JOSEPH HEREMANS, The Ohio State University — Thallium acts as a resonant level in PbTe, so that PbTe:Tl shows a significant improvement of thermoelectric properties due to an increase in thermopower as compared to that of similarly Na-doped PbTe [2]. Further improvements in ZT are expected from a reduction of the thermal conductivity by alloy scattering in Pb1−x−y TlxSnxTe and Pb1−x−y TlxTe1−xSey alloys. However, the band structure of PbTe is sensitive to alloying with Sn and Se, and thus the location of the Tl level with respect to the valence band can change with x. In this study, we investigate the effects that band structure modifications have on the enhancement of thermopower. Thermoelectric properties of Pb1−x−y TlxSnxTe and Pb1−x−y TlxTe1−xSey alloys with y=0.01-0.04 and x=0-0.3 are measured in directions longitudinal and transverse to magnetic fields in the range of 0.5-1.5 T. We report zero field values of electrical resistivity, thermopower, Hall coefficient and adiabatic Nernst-Ettingshausen coefficient as measured in temperature range 80-420K. From these we calculate carrier density and mobility and the density of states effective masses and Fermi energies. [2] J.P. Heremans et al., Science 321, 554 (2008)

5:06PM L28.00012 Enhancement of Thermoelectric Figure-of-Merit by a Nanostructure Approach, ZHIFENG REN, Boston College, BED POUDEL, GMZ Energy, Inc., YI MA, YUCHENG LAN, XIAOWEI WANG, GIRI JOSHI, GAOHUA ZHU, JIAN YANG, BO YU, XIAO YAN, HUI WANG, DEZHI WANG, Boston College, QING HAO, HOHYUN LEE, AUSTIN MINNICH, ANDREW MUTO, DARYOOSH VASHAEE, MILDRED DRESSELHAUS, GANG CHEN, MIT COLLABORATION, MIT COLLABORATION — The dimensionless thermoelectric figure-of-merit (ZT) in bulk materials has remained about 1 for many years. Here we show that a significant ZT improvement can be achieved in nanocrystalline bulk materials. These nanocrystalline bulk materials were made by hot-pressing nanopowders that are ball-milled from either crystalline ingots or elements. Electrical transport measurements, coupled with microstructure studies and modeling, show that the ZT improvement is the result of low thermal conductivity caused by the increased phonon scattering by grain boundaries and defects. More importantly, the nanostructure approach has been successfully applied to a few thermoelectric material systems, proving its generality. The approach can be easily scaled up to multiple tons. Thermal stability studies have shown that the nanostructures are stable at the application temperature for an extended period of time. It is expected that such enhanced materials will make the existing cooling and power generation systems more efficient.

Tuesday, March 17, 2009 2:30PM - 5:30PM –
Session L29 FEd DCOMP: Focus Session: Incorporating Computational Physics into Teaching

2:30PM L29.00001 One Lattice Gauge Theorist’s Perspective on Important Skills and Concepts for Computational Physics Courses, STEVEN GOTTLIEB, Indiana University — Lattice Gauge Theory employs a number of numerical and statistical techniques including: sparse matrix inversion, Monte Carlo methods, higher order numerical integration schemes, resampling methods such as jackknife and bootstrap, and parameter estimation from correlated data. Many of these techniques can be taught to undergraduates in contexts more easily understood than a lattice gauge theory simulation.

3:06PM L29.00002 Tips and Tools for Teaching Quantum Mechanics, GUANGTIAN ZHU, CHANDRALEKHA SINGH, Department of Physics & Astronomy, University of Pittsburgh — Learning quantum mechanics is challenging – students usually struggle to master the basic concepts, even though they may perform well on solving quantitative problems. Our group is investigating the difficulties that upper-level students have in learning quantum mechanics. To help improve student understanding of quantum concepts, we are designing quantum interactive learning tutorials (QuILTs) and tools for peer-instruction. Many of the tutorials employ computer simulations to help students visualize and develop better intuition about quantum phenomena. We will discuss the common students’ difficulties, share the material we have developed and evaluated to make the quantum mechanics class engaging and useful, and show ways to bridge the gap between quantitative and conceptual aspects of quantum mechanics.

3:18PM L29.00003 Building a Digital Library: Theory, Computation, and Education1, WOLFGANG CHRISTIAN, Davidson College — Over the past dozen years the Open Source Physics (OSP) project has produced some of the most widely used interactive curricular materials for high teaching of introductory and advanced physics courses. These materials are based on Java applets called Phsylets and on new OSP programs and applications. In this talk we will outline the pedagogical and technical features of these programs and describe our current effort to create and distribute our material using the comPADRE National Science Digital Library. Open Source Physics collection is available on the comPADRE website at http://www.compadre.org/osp/

1Partial funding for this work was obtained through NSF grant DUE-0442581.
Introducing scientific computation from high school to college: the case of Modellus

BRYNDOL SONES, FRANK WATTENBERG, US Military Academy — DIYModeling (Do it Yourself Modeling) aims to improve both the quality of learning in the STEM disciplines and the extent to which the very best STEM learning reaches all students by leveraging the power of game-quality modeling and simulation. It builds on earlier work by many people using platforms like Java, Flash and game-quality simulations like the Federation of American Scientists' Immune Attack. DIYModeling adds a new element that enables students and faculty to build their own game-quality simulations by specifying the underlying scientific and mathematical models without getting into the details of programming. The DIYModeling team is a consortium of math and basic science faculty from six universities teamed up with the software development company Tietronix Software (an 8a certified company), which does contract work for NASA to build complex software systems including game-quality immersive simulations. The goal of the program is to enable curriculum developers and students to develop game-quality, three-dimensional immersive simulations with educational benefit. Current applications under development include a first-person shooter game environment for use in data collection and statistical analysis, orbital mechanics in executing the Hohman transfer, and solar power generation. Some pilot tests are planned for use in the spring semester.

3:30PM L29.00004 Introducing scientific computation from high school to college: the case of Modellus

3:42PM L29.00005 DIYModeling: a place for students and faculty to build their own game-quality simulations to enhance learning.

EJS enhances traditional learning in freshman mechanics

AMY BUG, JEN TRINH, Swarthmore College — Easy Java Simulations (EJS) is a freeware authoring tool (part of the Open Source Physics project) [1]. EJS allows not only physics teachers, but students as well, to produce nonproprietary, platform-independent simulations with both numerical and graphical output. We report on the use of EJS as a helpful tool in a physics course for majors. In particular, EJS allows a student to conceptualize tough introductory material such as kinematics in polar coordinates and conservation of momentum with mass-transfer. The construction of an EJS simulation gives the student an environment in which to surmount both conceptual and mathematical roadblocks to learning. [1] http://www.opensourcephysics.org/

DIYModeling (Do it Yourself Modeling) aims to improve both the quality of learning in the STEM disciplines and the extent to which the very best STEM learning reaches all students by leveraging the power of game-quality modeling and simulation. It builds on earlier work by many people using platforms like Java, Flash and game-quality simulations like the Federation of American Scientists' Immune Attack. DIYModeling adds a new element that enables students and faculty to build their own game-quality simulations by specifying the underlying scientific and mathematical models without getting into the details of programming. The DIYModeling team is a consortium of math and basic science faculty from six universities teamed up with the software development company Tietronix Software (an 8a certified company), which does contract work for NASA to build complex software systems including game-quality immersive simulations. The goal of the program is to enable curriculum developers and students to develop game-quality, three-dimensional immersive simulations with educational benefit. Current applications under development include a first-person shooter game environment for use in data collection and statistical analysis, orbital mechanics in executing the Hohman transfer, and solar power generation. Some pilot tests are planned for use in the spring semester.

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3:54PM L29.00006 Computational Physics at Haverford College

Developing Computational Physics in Nigeria

GODFREY AKPOJOTOR, Max Planck Institute for Physics of Complex Systems, Dresden and Delta State University, Abakpa, EMMANUEL ENUKPERE, College of Education, Warri, FAMOUS AKPOJOTOR, Federal Government College, Sokoto, SUNNY OJOBOR, Delta State University, Abakpa — Computer based instruction is permeating the educational curricula of many countries owing to the realization that computational physics which involves computer modeling, enhances the teaching/learning process when combined with theory and experiment. For the students, it gives them more insight and understanding in the learning process and thereby equips them with scientific and computing skills to excel in the industrial and commercial environments as well as at the Masters and doctoral levels. And for the teachers, among others benefits, the availability of open access sites on both instructional and evaluation materials can improve their performances. With a growing population of students and new challenges to meet developmental goals, this paper examine the challenges and prospects of current drive to develop Computational physics as a university undergraduate programme or as a choice of specialized modules or laboratories within the mainstream physics programme in Nigeria institutions. In particular, the current effort of the Nigerian Computational Physics Working Group to design computational physics programmes to meet the developmental goals of the country is discussed.

4:18PM L29.00008 EJS enhances traditional learning in freshman mechanics

4:06PM L29.00007 Developing Computational Physics in Nigeria

4:30PM L29.00009 Computational Labs Using VPython Complement Conventional Labs in Online and Regular Physics Classes

MARTINA E. BACHLECHNER, Fairmont State University — Fairmont State University has developed online physics classes for the high-school teaching certificate based on the text book Matter and Interaction by Chabay and Sherwood. This lead to using computational VPython labs also in the traditional class room setting to complement conventional labs. The computational modeling process has proven to provide an excellent basis for the subsequent classroom lab and allows for a concrete experience of the difference between behavior according to a model and realistic behavior. Observations in the regular class room setting feed back into the development of the online classes.

We thank the Howard Hughes Medical Institute for funding.

4:42PM L29.00010 A New Graduate Minor Program in Computational Science

LYLE LONG, The Pennsylvania State University — This talk will discuss the need for graduate educational programs in computational science. Due to the continued increase in computer power, algorithms, and software the need for students trained in computational science has increased dramatically. Theoretical and experimental methods are still important, but there is an enormous need for students who understand numerical methods, programming, parallel computing, and software engineering. A new Graduate Minor program has been developed at Penn State and is now available to all graduate students (http://www.csci.psu.edu) The Ph.D. students are required to take two core courses (out of three possible), attend two seminar series, and choose two additional courses (which are often in engineering, science and college curricula, where computers are mainly used for showing text, images and animations. Most curricula do not consider the use of computational scientific tools, particularly tools where students can manipulate and build mathematical models, as an integral part of the learning experiences all students must have. In this paper, we discuss how Modellus, a freely available software tool (created in Java and available for all operating systems) can be used to support curricula where students from the age of 12 to college years can be introduced to scientific computation. We will also show how such a wide range of learners and their teachers can use Modellus to implement simple numerical methods and interactive animations based on those methods to explore advanced mathematical and physical reasoning.
A compound with one-dimensional chains of irregular edge-shared CoO$_2$ has shown that a spontaneous electric polarization of the order of 1.5 $\mu$C m$^{-2}$ develops below the magnetic transition temperature. This phenomenon is unique in that it exhibits spontaneous magnetization as well as electric polarization. We have studied the detailed switching behavior of magnetoelectric behaviors and suggest possible quantum phase transitions.

We have discovered the appearance of ferroelectricity below the Neel temperature of 6.7 K in the square-lattice antiferromagnetic Ba$_2$CoGe$_2$O$_7$, grown by using a floating zone technique. The ferroelectric polarization aligns along the tetragonal $c$ axis, but is very small in magnitude. However, the magnitude of polarization increases remarkably and the polarization direction smoothly rotates away from the $c$ axis with increasing magnetic fields along the $c$ axis. This change of polarization and the associated change of dielectric constant with fields are monotonic without going through any phase transition.

Ferroelectric magnets: a Conical Spiral and an Ising Chain. YOUNG JAI CHOI, Rutgers University — We have discovered the appearance of ferroelectricity below the Neel temperature of 6.7 K in the square-lattice antiferromagnetic Ba$_2$CoGe$_2$O$_7$, grown by using a floating zone technique. The ferroelectric polarization aligns along the tetragonal $c$ axis, but is very small in magnitude. However, the magnitude of polarization increases remarkably and the polarization direction smoothly rotates away from the $c$ axis with increasing magnetic fields along the $c$ axis. This change of polarization and the associated change of dielectric constant with fields are monotonic without going through any phase transition.

Ferroelectric magnets: a Conical Spiral and an Ising Chain. YOUNG JAI CHOI, Rutgers University — We have discovered the appearance of ferroelectricity below the Neel temperature of 6.7 K in the square-lattice antiferromagnetic Ba$_2$CoGe$_2$O$_7$, grown by using a floating zone technique. The ferroelectric polarization aligns along the tetragonal $c$ axis, but is very small in magnitude. However, the magnitude of polarization increases remarkably and the polarization direction smoothly rotates away from the $c$ axis with increasing magnetic fields along the $c$ axis. This change of polarization and the associated change of dielectric constant with fields are monotonic without going through any phase transition.

3:18PM  L30.00003 Electric polarization reversal under high magnetic field in square lattice antiferromagnetic Ba$_2$CoGe$_2$O$_7$. JAE WOOK KIM, S.H. CHUN, S.H. KIM, KEE HOON KIM, Seoul National University, Y. JO, L. BALICAS, NHHFL, Y.J. CHOI, S.W. CHEONG, Rutgers University, F. BALAKIREV, N. HARRISON, LANL. — Recently, Ba$_2$CoGe$_2$O$_7$, was found to develop electric polarization ($P$) below $T_N$=6.7 K [1]. Interestingly, $P$ along the $a$-axis increases linearly, crossing zero at $H$=0 when magnetic field ($H$) is applied along the $a$-axis. To investigate the linear $H$-dependence of $P$ further, we measured $P$ electric constant ($\epsilon$), and magnetization ($M$) under high $H$ up to 45 T. On application of high $H$, $P$ increases linearly up to $H$~15 T but suddenly decreases to a constant negative value. A peak in $\epsilon$ is found at the $P$-reversal point which is suppressed with increasing $H$ to lower temperature with a concomitant sharpening up to $H$~36 T at $T$=0.6 K. Furthermore, $M$/$H$ curves below $T_N$ show saturation above the $P$-reversal magnetic field, indicating that the negative $P$ state is due to the fully ordered spin configuration. This phenomenon is similar to the case of multiferroic BiMn$_2$O$_5$, in which $P$ reversal is driven by a spin-flop crossover [2]. However, in Ba$_2$CoGe$_2$O$_7$, $P$-reversal does not accompany a $H$ induced magnetic phase transition. We discuss possible mechanisms for this unique magnetoelectric behavior and suggest possible quantum phase transition behavior. [1] H. Yi et al., Appl. Phys. Lett. 91, 212904 (2008). [2] Jae Wook Kim et al., arXiv:0810.1907.

3:30PM L30.00004 Magnetic Frustution and Magnetoelastic Coupling in CoSe$_2$O$_5$. BRENT MELOT, RAM SESHADRI, Materials Department, UC Santa Barbara, AMBESH DIXIT, GAVIN LAWES, Department of Physics and Astronomy, Wayne State University, EMMANUELLE SUJARD, Institute Laue Langevin, Grenoble, France — We present structural and magnetic measurements on CoSe$_2$O$_5$, a compound with one-dimensional chains of irregular edge-shared CoO$_2$ octahedra, separated by Se$_2$O$_5$ units. Below 8.5 K low-field magnetic susceptibility and heat capacity measurements show long range antiferromagnetic order develops. The magnetic structure of this ordered state has been determined by neutron diffraction to consist of moments aligned antiparallel along the length of the chain as well as antiparallel to neighboring chains. The magnetic ordering becomes more complex when the compound is exposed under strong fields, with highly non-linear $M$~$H$ behavior below the ordering temperature. Measurement of the magnetoelectric constant and pyrocurrent has also shown directed fields larger than 3 T results in spontaneous electric polarization of the order of 1.5 $\mu$C m$^{-2}$ which develops below the magnetic transition temperature.
3:42PM L30.00005 Ferroelectricity from magnetic order. MICHELE KENZELMANN, Paul Scherrer Institute—Magnetic insulators with competing exchange interactions can give rise to strong fluctuations and qualitatively new ground states. The proximity of such systems to quantum critical points can lead to strong cross-coupling between magnetic long-range order and the chemical lattice. Case in point is a new class of multiferroic materials in which the magnetic and ferroelectric order parameters are directly coupled, and a magnetic field can suppress or switch the electric polarization [1]. Our neutron measurements reveal that ferroelectricity is induced by magnetic order and emerges only if the magnetic structure creates a polar axis [2-5]. Our experiments prove that the onset of ferroelectricity is described by a magneto-electric Landau theory that seems to apply for a wide range of multiferroic materials [6]. The spin dynamics and the field-temperature phase diagram of the ordered phases provide evidence that competing ground states are essential for ferroelectricity. The magneto-electric coupling, however, arising from relatively small interactions that are currently under intense investigation.


4:18PM L30.00006 Q-domains in Multiferroic CoCr$_2$O$_4$. THOMAS A. KAPLAN, Michigan State University—In spinel CoCr$_2$O$_4$, the observed spin at low temperature is, approximately, a “ferrimagnetic spiral” given by $S_{\nu} = \sin \theta_{\nu} [2 \cos (Q \cdot R_{\nu} + \gamma_{\nu}) + \hat{y} \sin (Q \cdot R_{\nu} + \gamma_{\nu})]$; $\gamma_{\nu}$ is the phase of the 6 conical spirals, all with wave vector Q in the [110] direction. This yields magnetization $M$ and, via the Katsura et al mechanism, electric polarization $P$. Equivalent Q’s, e.g. $\pm Q$, with associated M’s and P’s, are expected to give degenerate states, “$Q - M - P$ domains”; poling in electric and magnetic fields selects a single such domain. Reversal of magnetic field then leads to P reversal and Q reversal. But Q $\rightarrow$ $-Q$ in the equation above does not appear to give a degenerate state. I show, via the Heisenberg model and the Generalized Luttinger-Tisza method used in the prediction of the spin state, that $\gamma_{\nu} \rightarrow -\gamma_{\nu}$ on Q reversal, making manifest the Q $\rightarrow$ $-Q$ degeneracy.

1 M. Menyuk et al., J. de Physique 25, 528 (1964)
5 Y. Choi et al, submitted for publication

4:30PM L30.00007 Ginzburg-Landau theory for the conical cycloid state in multiferroics: Applications to CoCr$_2$O$_4$. CHUANWEI ZHANG, Department of Physics and Astronomy, Washington State University at Pullman, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, JOHN TONER, Department of Physics and Institute of Theoretical Science, University of Oregon at Eugene, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland at College Park—We show that the cycloidal magnetic order of a multiferroic can arise in the absence of spin and lattice anisotropies, e.g., in a cubic material, and this explains the occurrence of such a state in CoCr$_2$O$_4$. We discuss the case when this order coexists with ferromagnetism in a so-called “conical cycloid” state and show that a direct transition to this state from the ferromagnet is necessarily first order. On quite general grounds, the reversal of the direction of the uniform magnetization in this state can lead to the reversal of the electric polarization as well without the need to invoke “toroidal moment” as the order parameter.

1 This work is supported by NSF, NRI, LPS-NSA, and SWAN.

4:42PM L30.00008 Spin-driven ferroelectricity in triangular lattice antiferromagnets ACrO$_2$ ($A = Cu$, Ag, Li, or Na). SHINICHIRO SEKI, YOSHINORI ONOSE, YOSHINORI TOKURA, Department of Applied Physics, University of Tokyo — The correlation between the dielectric and magnetic properties is investigated on the triangular-lattice antiferromagnets ACrO$_2$ ($A = Cu$, Ag, Li, or Na) with the 120-degree spiral spin structure. For the $A = Cu$ and Ag compounds with defalosite structure, the ferroelectric polarization emerges with the spiral spin order, implying the strong coupling between the ferroelectricity and the spiral spin structure. For the $A = Li$ and Na compounds with ordered rock salt structure, on the other hand, no spontaneous polarization is discerned, while the clear anomaly in dielectric constant can be observed upon the transition to the spiral-spin ordered state. This feature can be ascribed to the possible antiferroelectric state induced by the alternate stacking of the Cr-spin chain with opposite vector spin chirality.

4:54PM L30.00009 Magnetoelectric coupling in a triangular lattice antiferromagnet CuCrO$_2$. KENTA KIMURA, HIROYUKI NAKAMURA, Osaka University, KEN'YA OHGUSHI, Institute for Solid State Physics, University of Tokyo, TSUYOSHI KIMURA, Osaka University—A triangular lattice antiferromagnet CuCrO$_2$ shows an out-of-plane 120° spin structure. Recently, ferroelectricity in the 120° phase has been reported for polycrystalline samples. However, no anisotropic information (e.g. direction of polarization) has been provided for lack of single-crystal measurement [1]. Therefore, we grew single crystals of CuCrO$_2$ and investigated their magnetic and ferroelectric properties [2]. We found that CuCrO$_2$ undergoes two successive magnetic phase transitions ($T_{N2}$ $\approx$ 24.2 K and $T_{N1}$ $\approx$ 23.6 K), probably into a collinear antiferromagnetic phase and then the out-of-plane 120° phase. Ferroelectric polarization within the triangular lattice plane appears only in the 120° phase. In the talk, we also discuss the magnetoelectric properties. [1] S. Seki et al., Phys. Rev. Lett. 101, 067204 (2008). [2] K. Kimura et al., Phys. Rev. B 78, 140401(R) (2008).

5:06PM L30.00010 Synthesis and properties of PbTi$_{1-x}$Ni$_x$O$_3$. LARRY BUROKER, SOMADITYA SEN, MARIJA GADJARDZISKA-JOSIFOVSKA, YING ZOU, SHISHIR RAY, MARK WILLIAMSEN, PRASENJIT GUPTASARMA, University of Wisconsin - Milwaukee, USA—Multiferroics are a class of multiferroic materials with magnetic and ferroelectric properties in the same phase. These have been a subject of intense investigation due to their fascinating physical properties, and the potential for new devices. We examine here the question of whether the successful substitution of a magnetic ion into a traditional ferroelectric lattice can result in a new magnetoelectric phase. Using a sol gel technique employing metal-ion chelate complexes, we have synthesized phase pure nanoparticulate samples of PbTi$_{1-x}$Ni$_x$O$_3$ for 0<x<0.3. We report our studies of crystal structure refinement, magnetic and dielectric properties 0.3<T<300 Kelvin, microstructure studies using High Resolution TEM, optical properties and vibrational spectroscopy in this new system.

1 Corresponding Author
5:18PM L30.00011 Impurity effects in multiferroic compounds, TRINANJAN DATTA, Augusta State University — We investigate the effect of impurities in multiferroic systems. Using an equation of motion approach for the spin dynamics of the host multiferroic compound, we find that the amplitude of the spin components of the material are affected by the impurities. We model the impurities as a two-level system and focus on the regime where the impurity spins relax slowly. When the impurity strength is weak the host spins oscillate with no decay and the electric polarization survives. However as the impurity strength is increased the host spin components get damped. This in turn causes the ferroelectricity to be destroyed. Since polarization in multiferroic materials is driven by magnetic ordering we conclude that the presence of impurities is detrimental to multiferroicity.

Tuesday, March 17, 2009 2:30PM - 4:54PM —
Session L31 GMAG DMP FLAP: Focus Session: Spin Transport and Exchange Bias in Nanostuctures 335

2:30PM L31.00001 Spin Injection and Accumulation in Metallic Lateral Spin Valves with Transparent Contacts1. FELIX CASANOVA, University of California San Diego — Creation and control of spin currents is a key ingredient in spintronics, which has as a goal the use of both the spin and charge of the electron. Ferromagnetic (FM)/non-magnetic (NM) lateral spin valves are powerful devices that decouple a pure spin current from an electrical current by using a non-local geometry. We will review previous works to show how the FM/NM interface and materials control in an essential way the generation and manipulation of a spin current in non-local spin valves (NLSV). For this reason, we have studied the electrical spin injection and spin accumulation in metallic NLSV with transparent interfaces as a function of important experimental parameters such as injection current direction and magnitude, temperature, materials, and thickness. Using injected DC currents we find that the spin injection is perfectly symmetric when injecting current from the FM or into the FM, causing exactly the opposite spin accumulation in the NM. This provides means for a pure electrical manipulation of the spin current polarity. The change in spin accumulation with increasing injected current is produced by a temperature raise of the device due to Joule heating and confirmed by independent spin accumulation measurements as a function of temperature. Comparing experimentally measured spin accumulation in NMs with a spin-diffusion model allows us to identify the effect of surfaces on the spin diffusion length and injection efficiency, and the effect of FM electrodes on spin accumulation. These experiments have important implications for the physics of NLSV and for the development of devices based on these phenomena.

1Work done in collaboration with A. Sharoni, M. Erekhtinsky and I. K. Schuller and supported by the US-DOE.

3:06PM L31.00002 Large-Room-Temperature Resistive Switching Behavior in Spinel Structured Nanoparticle Compacts. TAE HEE KIM, EUN YOUNG JANG, NYUN JONG LEE, Ewha Womans University, JUNG-TAK JANG, Yonsei University, JIN-SIL CHO, JINWOO CHEON, Yonsei University, KYUNG-JIN LEE, Korea University, EWHA WOMANS UNIVERSITY TEAM, YONSEI UNIVERSITY COLLABORATION, KOREA UNIVERSITY COLLABORATION — Here we report an abrupt and large bipolar switching behavior in the form of nanoparticle assembly consisting of an infinite number of monodispersed magnetic oxide single-crystallins. In the assembly of magnetite nanoparticles with size below 10 nm, we observed a room temperature voltage-current hysteresis with an abrupt and large bipolar resistive switching (switching ratio of ∼ 2000 %). We also found that such switching behaviors can be general phenomena for nanoparticle assemblies: not limited to magnetites but also consistently observed for other kinds of spinel structured nanoparticles with different compositions. Such a huge switching phenomenon it has never been observed before in bulk powders, particularly at room temperature. Our results showed clearly that the new I-V hysteresis is dependent on the nanoparticle size, and arises from interparticle contacts. In an effort to understand and interpret the origin of the bipolar reversible switching behavior, a new theoretical model was suggested in this work.

3:18PM L31.00003 Self-Assembly and Tunneling Magneto Resistance of Magnetic Nanoparticle Superlattices1. CHAITANYA LEKSHMI INDIRA, CONCETTA NOBILE, RAFFAELLA BOUNSANTI, ELIANA D’AMONE, DAVIDE COZZOLI, GIUSEPPE MARUCCIO, National Nanotechnology Laboratory, 73100 Lecce — Template assisted self-assembly of magnetic oxide nanostructures into systematically ordered superlattices in presence of magnetic field can offer controlled interfaces and useful properties for the fabrication of magnetically engineered tunnel junctions with application in high performance magnetic random access memories. In our work we employ magnetite, an important class of half-metallic material showing super paramagnetic behavior close to room temperature and low coercivity at low temperatures, as nanoparticles. The self-assembly of nanoparticle superlattices on metallic non-magnetic substrates is demonstrated. Further, enhanced spin-dependent electron transport and tunneling magneto resistance in devices with crossbar geometry is discussed.

1European Union Sixth Framework Programme

3:30PM L31.00004 Conductive atomic force microscopy measurements of nanopillar magnetic tunnel junctions. E. R. EVARTS, C. HOGG, Physics Dept, Carnegie Mellon University, J. A. BAIN, Electrical and Comp. Eng. Dept, Carnegie Mellon University, S. A. MAJETICH, Physics Dept, Carnegie Mellon University — Magnetic tunnel junctions have been studied extensively for their magnetoresistance and potential uses in magnetic logic and data storage devices, but little is known about how their performance will scale with size. Here we examined the electronic behavior of 12 nm diameter magnetic tunnel junctions fabricated by a novel nanomasking process. Scanning electron microscopy images indicated feature diameter of 12 nm, and atomic force microscopy showed a height of 5 nm suggesting that unmasked regions have been milled on average to the oxide barrier layer, and areas should have the remnants of the free layer exposed with no remaining nanoparticle. Electrical contact was made to individual nanopillars using a doped-diamond-coated atomic force microscopy probe with a 40 nm radius of curvature at the tip. Off pillar we observed a resistance of 8.1 x 106 Ω, while on pillar we found a resistance of 2.85 x 109 Ω. Based on the RA product for this film, 120 Ω - μm2, a 12 nm diameter cylinder with perfect contact would have a resistance of 1.06 x 109 Ω. The larger experimental value is consistent with a smaller contact area due to damaging the pillar during the ion milling process. The magnetoresistance characteristics of these magnetic tunnel junctions will be discussed.

3:42PM L31.00005 Spin filtering in transport through single-molecule magnet Mn12. KYUNGWHA PARK, Virginia Tech, Blacksburg, VA, SALVADOR BARRAZA-LOPEZ, Georgia Tech, Atlanta, GA, JAIME FERRER, Univ. of Oviedo, Spain, VICTOR GALVAÑA-SUÁREZ, U. de Oviedo, U. K. — We investigate electronic transport through a single-molecule magnet Mn12 in a two-terminal set up using the Green’s function method in conjunction with density-functional theory. Our transport calculation will provide crucial information on the effect of interfaces and molecular geometry on transport, and complement theoretical studies based on many-body model Hamiltonians. We consider a single-molecule magnet Mn12 bridged between Au electrodes via thiol group and alkane chains such that its magnetic easy axis is normal to the transport direction. The electrodes are treated semi-infinite and the transport calculation is performed self-consistently with density-functional theory. We present a spin-filtering effect through Mn12 and coupling strength of the Mn12 and electrodes. We also discuss the effect of additional electron correlations on the transport.
3:54PM L31.00006 Antiferromagnetic exchange coupling measurements on single Co clusters.
W. WERNSDORFER, CNRS, Institut Neel, Grenoble, D. LEROY, C. PORTEMONT, A. BRENAC, R. MOREL, L. NOTIN, CEA, INAC, Grenoble, D. MAILLY, LPN, CNRS, Marcoussis — We report on single-cluster measurements of the angular dependence of the low-temperature ferromagnetic core magnetization switching field in exchange-coupled Co/CoO core-shell clusters (4 nm) using a micro-bridge DC superconducting quantum interference device (µ-SQUID). It is observed that the coupling with the antiferromagnetic shell induces modification in the switching field for clusters with intrinsic uniaxial anisotropy depending on the direction of the magnetic field applied during the cooling. Using a modified Stoner-Wohlfarth model, it is shown that the core interacts with two weakly coupled and asymmetrical antiferromagnetic sublattices. Ref. : C. Portemont, R. Morel, W. Wernsdorfer, D. Mailly, A. Brenac, and L. Notin, Phys. Rev. B 78, 144415 (2008).

4:06PM L31.00007 The exchange bias effect in Ni/NiO and NiO nanoparticles1. ANGELA KOU, Harvard University, MIKHAIL FEYGENSON, LAUREN KRENO, Brookhaven National Laboratory. JONATHAN PATETE, AMANDA TIANO, FEN ZHANG, STANISLAUS WONG, SUNY at Stony Brook, MEIGAN ARONSON, Brookhaven National Laboratory — We used magnetic measurements, X-ray diffraction, and HRTEM to study the exchange bias field in Ni/NiO and NiO nanoparticles made by a modified wet chemistry method. We oxidized re-dispersed powders of bare Ni nanoparticles in air at 400°C and 900°C. HRTEM showed that annealing at 900°C of bare Ni nanoparticles led to the formation of exceptionally high quality NiO nanoparticles, resembling perfect bulk-like crystalline order. To our knowledge, there are no reports of NiO particles of such quality in the literature. The loop shift was 1000 Oe at 300K for the NiO nanoparticles, while it was only 120 Oe at 10K for the Ni/NiO nanoparticles. The difference is explained by the different origins of the loop shift in Ni/NiO and NiO nanoparticles. In Ni/NiO nanoparticles, the loop shift is associated with exchange interactions between ferromagnetic Ni and antiferromagnetic NiO. In NiO nanoparticles, however, the origin of the shift is an uneven number of ferromagnetic sublattices present in NiO nanoparticles, which interact differently with an applied magnetic field (Kodama, 1999).

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1Work at Brookhaven was funded by the U.S. Department of Energy.

4:18PM L31.00008 Correlation between bias fields and magnetoresistance in CoPt biased FeNi/Ta/FeNi GMR heterosystems, YI WANG, University of Nebraska-Lincoln, S. SAHOO, Seagate Technology. W. ECHTENKAMP, CH. BINEK, University of Nebraska-Lincoln — Exchange coupled magnetic hard layer (HL)/ soft layer (SL) thin films show SL biasing in close analogy to conventional exchange bias systems with antiferromagnetic pinning.1 Here we study CoPt(35nm)/FeNi450nm/Ta(d)/FeNi450nm heterostructures with d between 0.7 and 5nm. The CoPt films have in-plane magnetic anisotropy and pin the adjacent FeNi SL films. The latter are exchange coupled from top via Ta spacer layers with FeNi in a GMR-type architecture. We use AGFM and SQUID magnetometry to study the FeNi magnetization reversal with (CoPt) and without (vacuum) pinning layer proximity. The two minor FeNi hysteresis loops of the GMR trilayer reveal different biasing effects due to the distinct exchange interaction at the respective interfaces. The FeNi/CoPt coupling is systematically tuned via a series of set fields which allow partial demagnetization of the pinning layer. Moreover the comparison between the overall and minor magnetization reversals and the corresponding magnetoresistance effects for various temperature between T=20 and 400K.2 Ch. Binek, S. Poliysett, Xi He and A. Berger, Phys. Rev. Lett. 96, 067201 (2006). Financial support by NSF through Career DMR-0547887, MRSEC DMR-0820521 and the NRI.

4:30PM L31.00009 From Exchange Bias to Magnetic Memory, KARINE CHESNEL, BYU, Physics Dept, STEVE KEVAN, U Oregon, Physics Dept, ERIC FULLERTON, UCSD, MATT CAREY, Hitachi Global Storage, JEFF KORTRIGHT, LBNL, Material Sciences, BRIAN WILCKEN, JOSEPH NELSON, BYU — A better understanding and control of magnetic domain morphology and reversal processes in magnetic thin films is useful in the realm of perpendicular magnetic recording technology. We found the possibility to create magnetic domain memory in thin ferromagnetic films by inducing a spatially varying exchange coupling interactions. We evidenced this phenomenon in a perpendicular exchange bias film made of [Co/Pd] IrMn multilayers. Our coherent X-ray magnetic scattering speckle correlation study shows that the film exhibits no memory at room temperature but acquires a very high degree of magnetic memory, above 95% with subsequent field cycling when the sample is zero field cooled below the blocking temperature of the IrMn layers (Tc~275K).1 We present here the memory's dependency with magnetic field, temperature, and cooling conditions. We also discuss the spatial dependency by analyzing finely the local speckle correlation as a function of scattering angle, thus indicating variations of memory with different spatial scales in the domain pattern. [1] Chesnel et al, PRB, 78, 132409 (2008).

4:42PM L31.00010 Detection of Bottom Electrode Oxidation in Magnetic Tunnel Junctions via Exchange Bias Effect1. WEI CHEN, Department of Physics, University of Virginia, NAM DAO, KEVIN WEST, DAVID KIRKWOOD, JIWEI LU, STUART WOLF, Department of Materials Science and Engineering, University of Virginia, NANOSTAR TEAM — The oxidation of the bottom magnetic electrode (BE) in magnetic tunnel junctions (MTJs) is detrimental for high tunneling magnetoresistance (TMR). This has long been a tricky problem for the fabrication of MTJs. We propose a method to detect such oxidation by measuring the exchange bias effect from the CoO/ FM system if the BM surface is oxidized and CoO is formed. Along with the moderate exchange bias even more significant training effect and increased FM coercivity are observed at low temperature that depend on the oxidation level. All of these effects help in the detection of the FM surface oxidation. MTJs with MgO and vanadium oxide as tunnel barrier candidates are tested by this technique with the purpose of optimizing the barrier quality for best TMR performance.

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1This work is supported by DMEA under Contract No. H94003-08-2-0803 and ONR under Contract No. N00014-06-1-0428

Tuesday, March 17, 2009 2:30PM - 5:18PM —
Session L32 GMAG DMP: Focus Session: Nanostructured Manganites, Thin Films and Others

2:30PM L32.00001 Growth and characterization of the La0.67Sr0.33MnO3 nanowires. JUGDERSUREN BATTOGTOKH, 1, 2, SUNGMU KANG, 2, ROBERT S. DIPIETRO, DONALD HEIMAN, 3, ANDREW C. BUECHELE, 2, 1, 2, 3, 1DEPARTMENT OF PHYSICS, THE CATHOLIC UNIVERSITY OF AMERICA, WASHINGTON, DC 20064 TEAM. 2, VITREOUS STATE LABORATORY, THE CATHOLIC UNIVERSITY OF AMERICA TEAM. 3, DEPARTMENT OF PHYSICS, NORTHEASTERN UNIVERSITY, BOSTON, MA 02115. — Convolutional electrospinning method provides a simple approach to synthesis polymer nanowires. In this work, we report the growth, structural characterization, and magnetic properties of high-magnetic, ferromagnetic La0.67Sr0.33MnO3 (LSMO) alloy nanowires that are first time grown on Si/SiO2 substrates by the electrospinning method. Electrospun nanowires are annealed in an ultra-high purity argon-hydrogen gas mixture. Uniform, continuous, high aspect ratio LSMO nanowires with diameters in the range of 60–300 nm and lengths up to 500 µm are grown. The temperature dependent magnetization behavior of LSMO nanowires shows ferromagnetic behavior, and symmetric hysteresis loops are observed with magnetic fields applied to the substrate at 10 and 300 K. Finally, we will discuss the spin dependent electrical transport properties of the single LSMO nanowire.
2:42PM L32.00002 Resonant soft x-ray scattering from La$_{1-x}$Sr$_x$MnO$_3$ quantum wire arrays
SHUAI WANG, SERBAN SMADICI, JAMES LEE, MICHAEL ODLYZKO, XIAOFANG ZHAI, JAMES ECKSTEIN, AMISH SHAH, JIAN-MIN ZUO, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois, ANAND BHATTACHARYA, Argonne National Laboratory — Any finite sized, patterned system with an energy gap is expected to have elementary excitations that are characteristic of its boundary. To test this idea we have fabricated large arrays (> 60000 elements) of colossal magnetoresistance - phase La$_{2/3}$Sr$_{1/3}$MnO$_3$ quantum wires. These wires are 80 nm in width so have properties that are dominated by edge effects. We used resonant soft x-ray scattering (RSXS) and SQUID magnetometry to study their magnetic properties. We found that patterning lowers the Curie temperature and suppresses the degree of magnetization. RSXS studies show diffusion maxima from the wire period, as well as temperature-dependent diffuse scattering. We will discuss these results in the context of combined structural and magnetic disorder. Funding #: DOE grants DE-FG02-07ER46453 and DE-FG02-06ER46285

2:54PM L32.00033 Structure driven collapse of charge ordering in La$_{0.5}$Ca$_{0.5}$MnO$_3$ nanoparticles
A.K. RAYCHAUDHURI, TAPATI SARKAR, S.N. Bose National Centre for Basic Sciences, E. BOZIN, Columbia University, T. PROFFEN, Los Alamos National Laboratory, T. CHATTERJII, Inst.Laue - Langevin, S. BILLINGE, Columbia University — High resolution X-Ray and neutron diffraction had been used to show that size reduction below a certain size ( < 150nm) can lead to a collapse of the charge and orbitally ordered as well as the Antiferromagnetic ground state of the half doped manganese La$_{0.5}$Ca$_{0.5}$MnO$_3$. This leads to a ferromagnetic ground state. We show that the phenomena is linked to the structural changes that accompany the size reduction. The low temperature (T~15K) structure of the nanocrystals is significantly different from that of the bulk. The structure of the nanoparticles shows a distortion albeit different from that seen in the bulk which is driven by the Jahn - Teller distortion. The Rietveld analysis along with analysis of the Pair Distribution Function data show that there are differences in the way the MnO$_6$ octahedra are distorted in the bulk and the nanocrystals. We find that in the nanocrystals the structural distortion sets in at room temperature and shows very little variation on cooling. The Bragg peak of the ferromagnetic order in the nanoparticles was found to have the same indexes and approximately same d – spacing as that seen in ferromagnetic La$_{0.67}$Ca$_{0.33}$MnO$_3$.

3:06PM L32.00004 Jahn-Teller contribution to the magneto-optical response of ferromagnetic manganite thin films
GERSAVI HERRANZ, DAVID HRABOVSKY, JOSE MANUEL CAICEDO, INGRID CANERO-INFANTE, FLORENCIO SANCHEZ, JOSEP FONTCUBERTA, Institut de Ciencia de Materials de Barcelona, (ICMAB-CSIC) Bellaterra, Spain — We report on the temperature dependence of the magneto-optical response in the visible spectrum of ferromagnetic manganite thin films measured in transverse Kerr geometry. We show that this response is dominated by the usual magneto-optical Kerr effects for all temperatures except for a narrow window around the Curie temperature (T$_C$). Remarkably, the magneto-optical response of these manganite films does not die out near the ferromagnetic transition, in spite of the vanishing Jahn effect at those temperatures. On the contrary, the transverse Kerr response is hugely enhanced near T$_C$ and follows the same temperature dependence as the colossal magnetoresistance. We attribute these remarkable phenomena to the magnetic field-induced suppression of Jahn-Teller dynamical charge localization around T$_C$. Thus, the peculiar optical response of manganite films comes from the intricate physics of these strongly correlated electronic systems. We argue that the methodology we use is demonstrated to be very useful to understand the nature of some structural and electronic transitions driven by magnetic/electric fields or by temperature in other complex oxides.

3:18PM L32.00005 Observation of Ferromagnetic Resonance in SrRuO$_3$ Using the Time-Resolved Magneto-Optical Kerr Effect
M.C. LANGNER, C.L.S. KANTNER, Dept. of Physics, UC Berkeley and Lawrence Berkeley National Lab, Y.H. CHU, L.W. MARTIN, Dept. of Materials Science, UC Berkeley, R. RAMESH, Dept. of Physics and Dept. of Materials Science, UC Berkeley, J. ORENSTEIN, Dept. of Physics, UC Berkeley and Lawrence Berkeley National Lab — We report the observation of ferromagnetic resonance (FMR) in strontium ruthenate using the time-resolved magneto-optical Kerr effect. The FMR oscillations in the time-domain appear in response to a sudden, optically induced magnetic field. The frequency of these oscillations shows a weak dependence on temperature and other parameters associated with the magnetization dynamics, have a non-monotonic temperature dependence, suggestive of a link to the anomalous Hall effect.

3:30PM L32.00006 ABSTRACT WITHDRAWN

3:42PM L32.00007 ABSTRACT WITHDRAWN

3:54PM L32.00008 Switching Spectroscopy Piezoresponse Force Microscopy study of Domain Wall hysteresis at the nanoscale: Mapping lattice and defect pinning effects
VASUEVA RAO ARAVIND, Pennsylvania State University, SAMRAT CHOUDHURY, YULAN LI, KATYAYINI SEAL, STEPHEN JESSE, ANNA MOROZOVSKA, EUGENE ELISEEV, LONG-QING CHEN, SERGEI KALININ, VENKATRAMAN GOPALAN — In this work, using scanning probe microscopy with ~30 nanometer resolution along with theoretical modeling, we demonstrate the role of 180° ferroelectric domain wall as an intrinsic defect that lowers coercive fields in its vicinity by an order of magnitude. The interaction of ferroelectric 180° domain wall with a strongly inhomogeneous electric field of biased scanning probe microscope tip is analyzed within decoupling approximation allowing for the spatial redistribution of polarization caused by the biased probe using continuous Landau-Ginzburg-Devonshire theory. Theoretical calculations predict that equilibrium shape of the initially flat domain wall boundary bends, attracts or repels from the probe apex. The bending of the wall and its depolarization electric field facilitates tip induced domain nucleation. The experiments and theory are compared quantitatively, to show that lattice friction as well as lattice pinning play important role in the domain wall softening behavior. Acknowledgements: [1] National Science Foundation, [2] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory.

4:06PM L32.00009 Controlling Orthorhombic Domain Orientations in Epitaxial LaPrCaMnO Thin Films
JOHN BUDAI, Oak Ridge National Laboratory, T. ZAC WARD, Univ. of Tennessee, JON TISCHLER, JIAN SHEN, Oak Ridge National Laboratory — Microstructural effects such as strain and domain formation are known to influence the physical properties of transition metal oxide materials. For epitaxial films, lattice mismatch with the substrate can be used to investigate the effects due to in-plane biaxial tensile or compressive strain. Using synchrotron x-ray diffraction at the Advanced Photon Source, we have investigated the temperature-dependent lattice parameters and orthorhombic domain orientations for distorted pervoskite LaPrCaMnO thin films grown on several different substrates (SrTiO$_3$, LaAlO$_3$, SrLaGaO$_3$, NdGaO$_3$). We find that structural phase transition in the substrate can have a large effect on the film. More generally, we find that tensile and compressive stresses generate different orthorhombic domain orientations and can be used to control the microstructure of the LPCMO films .

1Support by DOE Office of Basic Energy Sciences, Div. of Materials Sciences & Engineering; XOR-UNI and APS supported by DOE-BES.
4:18PM L32.00010 Effect of the substrate on the orbital phase transition in a manganite thin film under magnetic field . Y. WAKABAYASHI, Osaka Univ., H. SAGAYAMA, T. ARIMA, Tohoku Univ., Y. NAKAMURA, Y. OGIMOTO, Tokyo Univ., K. MIYANO, Tokyo Univ., CREST, H. SAWA, Nagoya Univ. — Thin films of strongly correlated materials are studied intensively because of their potential of device application. Those materials in bulk form show various fascinating properties such as metal-insulator transition. However, clear phase transitions are often suppressed under the strain from the substrates. We have studied Nd$_{0.5}$Sr$_{0.5}$MnO$_3$ thin film on SrTiO$_3$ (011) substrate, which is a unique film that has clear orbital-ordering (OO) transition, by x-ray scattering under magnetic field up to 8T. As reported earlier [1], this system shows a net phase transition, paramagnetic (PM), ferromagnetic (F), A-type OO (A) to CE-type OO (CE) with cooling in zero field, and at F-A transition temperature (170K), the symmetry lowers and twin occurs. The phase sequence was changed to PM, F to CE above 4T, and above this field, considerable amount of the FM phase remains down to 10K. This field induced phase separation is attributable to the martensitic accommodation strain at the domain boundary. [1] Y.W. et al., Phys. Rev. Lett. 96 017202 (2006), J.Phys.Soc.Jpn. 77, 014712 (2008).

4:30PM L32.00011 Coherent Long Range Lateral Charge Ordering in strained Epitaxial Oxide Film Structures. JONG-WOO KIM, PHILIP, RYAN, Ames Laboratory, JAK, CHAKHALJAN, MIKHAIL, KAREEV, JIAN LIU, University of California, San Diego, STEVE MAY, ANAND BHATTACHARYA, JOHN FREELAND, Argonne National Laboratory, AMES LABORATORY COLLABORATION, UNIVERSITY OF ARKANSAS COLLABORATION — The quality of ordered oxide films has reached the level whereby epitaxial superlattice structures can now be achieved by both pulsed laser deposition (PLD) and ozon assisted molecular beam epitaxy (MBE) growth. Engineering each layer coupled with compressive and tensile strain with the explicit aim of controlling and or enhancing the macroscopic electrical and magnetic ordering is a considered aim of ordered oxide film growth. The question how highly strained films structurally respond to such stress is examined by synchrotron diffraction. Both LaSrMnO films grown on STO(001) by MBE and PLD grown LaNAlO films on both LAO(001) and STO(001) have revealed coherent lateral order dependent upon film disorder, substrate mismatch induced strain and even dislocations induced by the substrate step morphology.

4:42PM L32.00012 Dember effect induced photovoltage in perovskite p-n heterojunctions. KUI-JUAN JIN, KUN ZHAO, HUI-BIN LU, LENG LIAO, GUO-ZHEN YANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, CAS, Beijing 100080, China — An unusual and rather large transient lateral photovoltage (LPV) has been observed in La$_{0.9}$Sr$_{0.1}$MnO$_3$/SrNb$_{0.01}$Ti$_{0.99}$O$_3$ and La$_{0.7}$Sr$_{0.3}$MnO$_3$/Si heterojunctions under the nonuniform irradiation of pulsed laser. The irreversible LPVs on both sides of a p-n junction challenge the well established model for LPV in conventional semiconductor p-n junctions, which can be well explained by Dember effect. Much larger LPV is observed in La$_{0.7}$Sr$_{0.3}$MnO$_3$/Si than that in La$_{0.9}$Sr$_{0.1}$MnO$_3$/SrNb$_{0.01}$Ti$_{0.99}$O$_3$. Similar results measured from both substrates of SrNb$_{0.01}$Ti$_{0.99}$O$_3$ and Si also support such a Dember effect. Much larger LPVs in heterojunctions than those in simple samples (SrNb$_{0.01}$Ti$_{0.99}$O$_3$ or Si) suggest a potential application of Dember effect in heterostructures.

5:06PM L32.00014 Spins and Twins: Correlation between Crystallographic and Magnetic Domains at Co/NiO(001) Interfaces. HENDRIK OHLDAG, SSRL, Menlo Park CA, USA., ELKE ARENHOLZ, ALS, Berkeley CA, USA., GERRIT VAN DER LAAN, Diamond Light Source, Chilton UK — Using soft x-ray spectromicroscopy we show that NiO(001) exhibits a crystallographic and ordering dependent upon film disorder, substrate mismatch induced strain and even dislocations induced by the substrate step morphology.

5:06PM L32.00014 Spins and Twins: Correlation between Crystallographic and Magnetic Domains at Co/NiO(001) Interfaces. HENDRIK OHLDAG, SSRL, Menlo Park CA, USA., ELKE ARENHOLZ, ALS, Berkeley CA, USA., GERRIT VAN DER LAAN, Diamond Light Source, Chilton UK — Using soft x-ray spectromicroscopy we show that NiO(001) exhibits a crystallographic and ordering dependent upon film disorder, substrate mismatch induced strain and even dislocations induced by the substrate step morphology.

Tuesday, March 17, 2009 2:30PM - 5:30PM –
Session L33 DCMP: Superconductivity: Electronic Structure I 403

2:30PM L33.00001 IR Hall measurements in overdoped Pr$_{2-x}$Ce$_x$CuO$_4$: evidence for magnon induced current-vertex corrections . GREGORY S. JENKINS, DON C. SCHMADEL, R.L. GREENE, H.D. DREW, University of Maryland at College Park, P. FOURNIER, Universite de Sherbrooke, H. KONTANI, Nagoya University — In overdoped Pr$_{2-x}$Ce$_x$CuO$_4$, the dc Hall coefficient achieves its expected value $R_H \propto 1 + x$ consistent with the large hole-like Fermi surface observed in ARPES, but only at low temperatures. As temperature is raised, the dc Hall coefficient falls off and becomes negative at a temperature that increases with $x$. We have measured the IR Hall angle of two overdoped Pr$_{2-x}$Ce$_x$CuO$_4$ samples at sufficiently low optical excitation energies (below 10meV) to directly probe the Fermi-surface properties. The observed large deviations from the classical result correspond to the addition of electron-like contributions to $\sigma_{xy}$, even at $T=0$, due to the finite frequency. Results of a model developed by H. Kontani of the low frequency IR Hall response which incorporates current-vertex corrections induced by magnon scattering are directly compared to the data. The model fully captures the salient features of the measured Hall response as a function of doping, temperature, and frequency. These results demonstrate that the anomalous Hall effect in the cuprates is a consequence of current vertex corrections to $\sigma_{xy}$.

1We acknowledge the support of CNAM and NSF.
2:42PM L33.00002 Fermi surface reconstruction in e-doped cuprates: IR Hall measurements in underdoped \( Pr_{2-x}Ca_xCuO_4 \), D.C. SCHMADELE, G.S. JENKINS, H.D. DREW, R.L. GREENE, Center for Nanophysics and Advanced Materials, University of Maryland at College Park, P. FOURNIER, Universite de Sherbrooke — The complex IR Hall angle is measured in PCCO at doping levels ranging from 10% to 15% at low optical excitation energy (10 meV). A precipitous decrease in Hall mass with a decrease in doping level in the underdoped regime is strong evidence of Fermi surface reconstruction and pocket formation, an observation consistent with ARPES and optical spectroscopy measurements. The data over the entire underdoped region is consistent with the predicted IR Hall response based upon ARPES data and Boltzmann theory. The temperature dependence of the Hall mass indicate a gradual roll-over from small pockets to the large unreconstructed Fermi surface expected in overdoped PCCO.

1We acknowledge the support of CNAM and NSF.

2:54PM L33.00003 Evidence for Fermi surface reconstruction in h-doped cuprates: IR Hall measurements in underdoped \( La_{2−x}Sr_xCuO_4 \), H.D. DREW, G.S. JENKINS, D.C. SCHMADELE, R.L. GREENE, Center for Nanophysics and Advanced Materials, University of Maryland at College Park, ICHIRO TSUKADA, Central Research Institute of Electric Power Industry, Japan — We measure the IR Hall angle in \( La_{2−x}Sr_xCuO_4 \) as a function of doping ranging from 7% to 16.5%. The optimally doped sample is shown to be consistent with ARPES measurements of the Fermi arcs in ARPES experiments is observed. The rapid decrease in Hall mass with underdoping is a hallmark signature of Fermi surface reconstruction exhibited in systems which are well known to fractionalize into Fermi pockets (underdoped PCCO). Comparisons with Fermi surface models will be discussed.

We acknowledge the support of CNAM and NSF.

3:06PM L33.00004 Quantum Oscillations in the Specific Heat of Ultraclean YBCO in 45T magnetic fields, SCOTT RIGGS, NHMFL/FSU, JON BETTS, LANL, SUCHITRA SEBASTIAN, Cambridge, NEIL HARRISON, ALBERT MIGLIORE, LANL, GREG BOEBINGER, NHMFL/FSU, RUIXING LIANG, WALTER HARDY, DOUG BONN, Simon Fraser University — We report specific heat measurements of Ortho-II YBCO in a magnetic field as large as 45T to directly compare the superconducting state with the normal state at low temperatures. This thermodynamic measurement of the electronic density of states determines the total number of carrier pockets in the two-dimensional Fermi surface of Ortho-II YBCO. These measurements also reveal quantum oscillations in the specific heat that provide a bulk measurement of the quasiparticle density of states in the d-wave mixed state.

3:18PM L33.00005 De Haas-Van Alphen Experiments on BaNi_2P_2, TAICHI TERASHIMA, MOTOI KIMATA, HIDETAKA SATSUKAWA, ATSUSHI HARADA, KAORI HAZAMA, MOHORU IMAI, SHINYA UJI, National Institute for Materials Science, Japan, HIJIRI KITO, AKIRA IYO, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology (AIST), Japan, HISATOMO HARIMA, Kobe University, Japan — We have observed de Haas-van Alphen (dHvA) oscillations in BaNi_2P_2, which is isostruktrual with BaFe_2As_2 and becomes superconducting below \( T_c = 3 \) K without doping [T. Mine et al., Solid State Commun. 147, 111 (2008)]. It is a suitable compound to study how different electronic structures are between iron and nickel-based superconductors. The single crystals used in the study were obtained by high-pressure synthesis. dHvA frequencies up to 8 K were observed, and their size and angular dependences can be explained very well by a band-structure calculation. Effective masses are two to three times larger than the corresponding band masses, suggesting moderate mass enhancement due to electron-phonon-electron interactions.

3:30PM L33.00006 de Haas van Alphen Effect in Strongly Interacting Systems, LARA THOMPSON, University of British Columbia, P.C.E. STAMP, UBC, PITP — We present calculations of de Haas van Alphen (dHvA) oscillations for strongly interacting systems, for (1) systems near a quantum phase transition (QPT); and/or (2) 2D and quasi-2D systems. The standard Lifshitz-Kosevich (LK) results are then inapplicable. D Hva, the quantum interaction scale goes to zero, giving strong corrections to LK. In 2D, LK breaks down entirely in the presence of interactions. Recently, dHvA oscillations in high Tc systems have been measured, but their form does not yet rule out non-Fermi liquid behaviour. We calculate the expected magnetization response assuming various Fermi reconstruction scenarios. The response depends crucially on the inter-plane couplings, and we find deviations from LK if the reconstruction is interaction-driven.

3:42PM L33.00007 Interpreting the Gap Signatures in the Raman Spectra of Hg-1201, JAMES STOREY, University of Cambridge, JEFFERY TALLON, Industrial Research Limited — Recently, peaks in the B1g and B2g Raman spectra of the Hg-1201 high-Tc cuprate superconductor have been interpreted in terms of two gaps. These are i) a gap near the Brillouin zone boundary that decreases monotonically with doping, and ii) a gap near the zone diagonal that follows the dome-shaped doping dependence of the superconducting transition temperature. The former has come to be interpreted as the pseudogap and the latter the superconducting gap. However, this dome shaped superconducting gap contradicts ARPES evidence for the existence of Ca 3d derived states at \( E_F \), which probably play a crucial role for the unusually superconductivity. The electronic structure of CaC_6 is compared with the electronic structures of other graphite intercalation compounds, providing deeper understanding of the superconductivity of CaC_6.

1Supported by the Marsden Fund of New Zealand.

4:06PM L33.00009 The existence of substantial Ca 3d derived states at \( E_F \) in Ca-intercalated graphite superconductor CaC_6, HIROYUKI OKAZAKI, RIKIYA YOSHIDA, KEISUKE IWAI, KENGO NOAMI, Okayama University, TAKAYUKI MIRO, TETSUYA NAKAMURA, JASRI/SPring-8, TAKANORI WAKITA, YUJI MURAOKA, MASAKI HIROI, Okayama University, FUMIYAKI TOMIOKA, YOSHIKO TAKANO, NIMS, ASAMI TAKENAKA, MASASHI TOYODA, Oita University, TAMIO OGUCHI, Hiroshima University, TAKAYOSHI YOKOYA, Okayama University — We have performed soft x-ray photoemission studies of Ca-intercalated graphite superconductor CaC_6 (\( T_c = 11.2 \) K). The valence band spectrum shows six main structures that correspond to those of calculated DOS that predicts large Ca 3d contribution at the Fermi level (\( E_F \)). The Ca 2p core level spectrum has a very large asymmetric line shape, suggesting the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites. These results provide spectroscopic evidence for the existence of Ca 3d derived conduction electrons at Ca sites.

1This work was partially supported by KAKENHI and JST-CREST.
4:18PM L33.00010 Orbital excitation in Sr$_2$CuO$_2$Cl$_2$ resonant inelastic x-ray scattering at the Cu K pre-edge. JUNGHO KIM, D. S. ELLIS, T. GOG, D. CASA, YOUNG-JUNE KIM, CMC-CAT, APS. ARCONNE NATIONAL LAB. COLLABORATION, UNIVERSITY OF TORONTO COLLABORATION — d − d excitations has attracted much attention due to its fundamental importance in elucidating electronic structure. However, experimental study of these excitations is difficult, since direct optical transition is dipole forbidden. We show that the Cu 1s-3d intermediate state, which can be reached via electric quadrupole operator, provides an excellent high-resolution means for studying d − d excitations in cuprates, and complements other well established techniques. Since quadrupole operator is sensitive to the symmetry of the intermediate state, considerable information on the symmetry of d − d excitation can be gained by exploiting this resonance. We have carried out comprehensive angle resolved x-ray absorption spectroscopy experiment, which clearly demonstrates the quadrupole nature of the absorption. We find that our RIXS spectra at this quadrupole resonance exhibit a broad excitation centered at 2 eV. We suggest that the scattering angle dependence of the quadrupole resonance agrees well with the calculated polarization dependence of quadrupole matrix element and information on the symmetry of d − d excitation can be obtained. Our analysis show that the quadrupole resonance at 2eV is consistent with the excitation involving 3d$^9_{y^2-x^2}$ symmetry.

4:30PM L33.00011 Quantum oscillation experiments on YBa$_2$Cu$_3$O$_{6.60}$1. JOHN SINGLETON, ROSS MC DONALD, SUSAN COX, National High Magnetic Field Laboratory, SHILIANG LI, PENGCHENG DAI, Physics, University of Tennessee — Pulsed magnetic fields of up to 75 T and temperatures down to 0.40 K have been used to study single crystals of YBa$_2$Cu$_3$O$_{6.60}$. The samples are measured using a MHz technique that is sensitive to small changes in penetration depth in the superconducting state, and to changes in the skin depth in the normal state. Two series of magnetic quantum oscillations are observed, sensitive in periodic in inverse field; the frequencies are 590 ± 20 T and 1990 ± 40 T. This suggests that the predicted large Fermi surface is broken into smaller pockets due to nesting. These findings are discussed in the context of other recent observations of quantum oscillations in the cuprates, and a magnetically-mediated mechanism for superconductivity, driven by the topological mapping of the d-wave Cooper-pair wavefunction onto the antiferromagnetic fluctuations (due to Fermi-surface nesting) that are observed across the whole cuprate phase diagram (R.D. McDonald et al., J. Phys.: Condens. Matter, in press (2008)).

1Supported by DoE grant “Science in 100 T”.

4:42PM L33.00012 Five Principles of Photoemission of High Temperature Superconducting Cuprates Deduced from the Diplon Theory. RAM SHARMA, University of Illinois at Chicago, IL. — In the process of the theoretical explanation of the observed photoemission result of high temperature superconducting cuprates we have been able to derive by means of the diplon theory [1,2] five principles of photoemission in various situations of doping, temperature and Fermi level crossing. These five principles interrelate the peak-dip-hump phenomenon, the kink structure (including the predicted high energy kinks [3]) in the quasiparticale energy dispersion and electron velocities at different energies with respect to the characteristic diplon excitations in the system. Details of the five principles will be presented. The theory contains Mott renormalization and all important and necessary electron-electron correlations.


5:06PM L33.00014 Using photoemission spectroscopy to probe a strongly interacting Fermi gas1. JOHN STEWART, JOHN GAEBLER, DEBORAH JIN, JILA-University of Colorado — We use photoemission spectroscopy to directly probe the elementary excitations and energy dispersion of a strongly interacting Fermi gas of atoms. In these photoemission experiments, an rf photon ejects an atom from our strongly interacting system via a spin-flip transition to a weakly interacting state. This new measurement technique for ultracold atom gases, like photoemission spectroscopy for electronic materials, directly probes low energy excitations and thus can reveal excitation gaps and/or pseudogaps. We observe a back-bending of the excitation spectrum consistent with a BCS-like dispersion curve.

1JILA, Quantum Physics Division, National Institute of Standards and Technology and Department of Physics, University of Colorado, Boulder, CO 80309-0440, USA.

5:18PM L33.00015 Ab initio calculation of core-valence-valence Auger spectra in closed shell systems. GIAN PAOLO BRIVIO, GUIDO FRATESI, MARIO ITALO TRIONI, Universita' di Milano-Bicocca, SIMONA UGENTI, ENRICO PERFETTO, MICHELE CINI, Universita' di Roma Tor-Vergata, MILANO-BICOCCA COLLABORATION, ROMA TOR-VERGATA COLLABORATION — We propose an ab initio method to evaluate the core-valence-valence Auger spectrum of systems with filled valence bands. The method is based on the Cini-Sawatzky theory, and aims at estimating the parameters by first-principles calculations in the framework of DFT. Photoemission energies and the interaction energy for the two holes in the final state are evaluated by performing DFT simulations for the system with varied population of electronic levels. Transition matrix elements are taken from atomic results. The approach takes into account the non spherical density of states of the emitting atom, spin-orbit interaction in core and valence, and non quadratic terms in the total energy expansion with respect to fractional occupation numbers. It is tested on two benchmark systems, Zn and Cu metals, leading in both cases to 2234/4514 Auger peaks within 2 eV from the experimental ones. Especially problematic is the evaluation of the hole-hole interaction for systems with broad valence bands: our method understimates its value in Cu, while we obtain excellent results for this quantity in Zn.
usual flux pinning effects and bistable superconductivity. We will firstly consider geometry hybrids exhibit a plethora of induced effects and novel physical properties, due to the interplay between the competing S and F orders. We will show a few examples of those, in a series of experiments on a simple hybrid system: a thin film with an array of F nanodots. Changing the array geometry, the nanodots size or their magnetic state allows to investigate a large variety of physical phenomena. We will focus on two of them: flux pinning effects and stray-magnetic-field induced manipulation of superconductivity. We will firstly consider geometry induced effects; in particular, we will compare the pinning properties of periodic, quasiperiodic, and fractal arrays. Secondly, we will discuss the effects induced by particular nanodot magnetic-states. We will show experiments on the interaction between flux quanta and nanodot magnetic vortices, which can be used to obtain switchable flux pinning potentials. Finally, we will describe an experiment in which the magnetic reversal events of the nanodot magnetic vortices are imprinted into the transport properties of a superconducting thin film. This yields a very unusual hysteretic magnetoresistance. This effect is induced by the stray magnetic fields from the nanodots, which drive the superconducting-to-normal transition of the hybrid depending on the magnetic history.


In collaboration with C. -P. Li, K. D. Smith, M. I. Montero, R. Morales, L. Huang, Y. Zhu and Ivan K. Schuller. Work supported by NSF and US-AFOSR.

3:06PM L34.00002 Vortex ratchet effect induced by different magnetic configurations in magnetic superconducting hybrids. D. PEREZ DE LARA, Universidad Complutense de Madrid(UCM), F.J. CASTANO, Massachusetts Institute of Technology(MIT), B.G. NG, MIT, R.K. DUMAS, University of California Davis(UC-Davis), E.M. GONZALEZ, UCM, KAI LIU, UC- Davis, C.A. ROSS, MIT, IVAN K. SCHULLER, University of California-San Diego, J.L. VICENT, UCM — We have used E-Beam Lithography to prepare hybrid systems consisting of arrays of nanometric Ni rings (elliptical and circular) covered by a superconducting Nb film. These nanometric rings were characterized by a First Order Reversal Curve method to realize the onion and vortex magnetic state at remanence. The transport properties of the superconducting Nb film were measured in the mixed state by applying a magnetic field perpendicular to the sample. Classical pinning matching effects of very high order were observed in resistance vs H, which vary with the magnetic state of Ni rings. Interestingly, a ratchet effect characterized by a dc output voltage produced by an applied ac current is found. Moreover, the ratchet effect is drastically modified by the remanent magnetic state of the Ni rings. The systematic and origin of the ratchet effect will be discussed.

This work was supported by Spanish Ministerio de Ciencia e Innovacion, grants FIS2008-06249, NAN2004-09087, FIS2005-07392, Fondo Social Europeo, AFOSR and CITRIS

3:18PM L34.00003 Antivortex complexes and intrinsic ratchet dynamics in superconductors with progressive magnetic topology. ANDRAS LIBAL, MILORAD MILOSEVIC, Departement Fysica, Universiteit Antwerpen, Belgium, FRANCOIS PEETERS, Departement Fysica, Universiteit Antwerpen, Belgium, W. GILLIJNS, A.V. SILHANEK, V.V. MOSCHALKOV, INPAC - Institute for Nanoscale Physics and Chemistry, Katholieke Universiteit Leuven, Belgium — Theoretically and experimentally, we analyze characteristic properties of a superconducting (Sc) film deposited on parallel arrays of ferromagnetic (Fm) dots with gradually increasing diameter in a periodic saw-tooth manner. Due to their perpendicular magnetization, dots induce vortex-antivortex molecules in the sample, with number of constituent (anti) vortices growing with magnet size. Resulting gradient of antivortex density between the dots predetermines local nucleation of superconductivity in the sample as a function of applied external field and temperature. In applied drive however, antivortices act collectively in an asymmetric potential of the dots and pinned vortices, and exhibit unique ratchet dynamics intrinsic to the Sc-Fm hybrids.

1. Work supported by the Flemish Science Foundation (FWO-VI), the Belgian Science Policy, the K.U.L. Research Fund GOA/2004/02, and the JSPS/ESF-ESF program. A.L., W.G., and A.V.S. acknowledge individual support from FWO-VI.

2:30PM L34.00004 Vortex dynamics and vortex lattice reconfiguration in superconducting-magnetic hybrids. JOSE L. VICENT, DAVID PEREZ DE LARA, Universidad Complutense, ALEJANDRO ALIJA, Universidad Oviedo, ELVIRA M. GONZALEZ, Universidad Complutense, JOSE I. MARTIN, MARIA VELEZ, Universidad Oviedo, JOSE V. ANGUITA, Instituto Microelectronica (CSIC) — Amorphous superconducting films (M02/Si) have been grown on top of array of nanometric magnets. These periodic magnetic centers have been fabricated on Si substrates by Electron Beam Lithography and sputtering techniques. In the mixed state the competition between the intrinsic and random pinning potential of the superconducting film and the artificial induced periodic pinning potential governs the vortex lattice behavior. Close to critical temperature, the periodic potentials could overcome the random potentials, then the vortex lattice dynamics shows effects which are related with the array dimension and symmetry. We will show in these hybrid systems enhancements of matching effects between the vortex lattice and the array unit cell, and different vortex lattice configurations.

3:00PM L34.00005 Scanning Tunneling Spectroscopy Study of Proximity Effect in Bilayer Manganese/Cuprate Thin Films. I. FRIDMAN, J.Y.T. WEI, University of Toronto, L. GUNAWAN, G.A. BOTTON, McMaster University — Recent work has suggested novel proximity and spin diffusion effects in ferromagnet/superconductor heterostructures composed of transition-metal perovskites. We have performed scanning tunneling spectroscopy (STS) on La0.75Ca0.25MnO3/YBa2Cu3O7−δ (LCMO/YBCO) bilayer thin films. Films were epitaxially grown on <001> SrTiO3 substrates using pulsed laser deposition with either the LCMO or YBCO layer on top. The STS data taken at 4.2 K were analyzed for spectral signatures of a pairing gap on the LCMO layer and spin diffusion in the YBCO layer, and to determine the length scale of the proximity effect and the role played by magnetic domain walls.

Work supported by NSERC, CFI/OIT and the Canadian Institute for Advanced Research.
Josephson junctions — We apply the scattering matrix approach to the triplet proximity effect in superconductor-half metal structures. We find that for junctions that do not mix different orbital modes, the zero bias Andreev conductance vanishes, while the zero bias Josephson current is nonzero. We illustrate this finding on a ballistic half-metal/superconductor (HS) and superconductor/half-metal/superconductor (SHS) junction with translation invariance along the interfaces, and on HS and SHS systems through the half-metallic region takes place through a single conducting channel. Our calculations for these physically single mode setups single mode point contacts and chaotic quantum dots with single mode contacts illustrate the main strength of the scattering matrix approach: it allows for studying systems in the quantum mechanical limit, which is inaccessible for quasiclassical Green’s function methods, the main theoretical tool in previous works on the triplet proximity effect.

4:06PM L34.00007 Reentrant resistance in mesoscopic superconductor-ferromagnet-superconductor structures1. MADALINA COLCI, MARTIN STEHNO, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — We report measurements of the resistance as a function of temperature and magnetization alignment in hybrid structures consisting of superconducting electrodes connected by two ferromagnetic nanowires separated by less than a superconducting coherence length. It has been predicted that such structures could exhibit a supercurrent due to Cooper pair splitting and coherent transport through the ferromagnets. Although we have not observed a zero-voltage supercurrent, we find that as the temperature is lowered below the critical temperature of the superconductor, the resistance of the structure shows a minimum and then rises, suggestive of re-entrant behavior. The resistance of the superconducting array of ferromagnetic wires is found to be lower than in the parallel case just below Tc but becomes distinctly larger than in the parallel case at the lowest temperature. We discuss possible explanations and implications of this result.

1Work supported by NSF grant DMR06-05813

3:54PM L34.00006 Quantum limit of the triplet proximity effect in half-metal - superconductor junctions. JOERN K. KUPFERSCHMIDT, LASSP, Cornell University, B. BERI, C.W.J. BEENAKKER, Instituut-Lorentz, Universiteit Leiden, P.W. BROUWER, LASSP, Cornell University — We apply the scattering matrix approach to the triplet proximity effect in superconductor-half metal structures. We find that for junctions that do not mix different orbital modes, the zero bias Andreev conductance vanishes, while the zero bias Josephson current is nonzero. We illustrate this finding on a ballistic half-metal/superconductor (HS) and superconductor/half-metal/superconductor (SHS) junction with translation invariance along the interfaces, and on HS and SHS systems through the half-metallic region takes place through a single conducting channel. Our calculations for these physically single mode setups single mode point contacts and chaotic quantum dots with single mode contacts illustrate the main strength of the scattering matrix approach: it allows for studying systems in the quantum mechanical limit, which is inaccessible for quasiclassical Green’s function methods, the main theoretical tool in previous works on the triplet proximity effect.

4:18PM L34.00008 Ferromagnets without inversion symmetry - room for superconductivity?1. ANDRIY NEVIDOMSKY, Rutgers University, JACOB LINDER, ASLE SUDBø, Norwegian University of Science and Technology, Trondheim, Norway — Motivated by the recent discoveries of ferromagnetic and non-centrosymmetric superconductors, we present a mean-field theory [1] for a superconductor that both lacks inversion symmetry and displays ferromagnetism, a scenario which is believed to be realized in UIr under applied pressure [2]. We study the interplay between the order parameters to clarify how superconductivity is affected by the presence of ferromagnetism and spin-orbit coupling. We find that the spin-orbit coupling seems to enhance both ferromagnetism and superconductivity in both singlet and triplet channels. We discuss our results in the context of the heavy fermion superconductor UIr and analyze possible symmetries of the order parameter.


3:42PM L34.00010 Splitting of a Cooper pair by a pair of Majorana bound states. JOHAN NILSSON, Instituut-Lorentz, Leiden University — Majorana fermions are spatially localized superpositions of electron and hole excitations in the middle of a superconducting energy gap. These unusual particles have been predicted to occur at the interface between a magnetic and a superconducting electrode, in contact with a topological insulator (such as a BiSb crystal or a HgTe quantum well). A single qubit can be encoded nonlocally in a pair of spatially separated Majorana fermions. We have measured the critical current of Josephson junctions of the form Nb/Co/Ru/Co/Nb, where the two Co layers are exchange-coupled antiferromagnetically by an intrinsic flux cancellation. The junctions were fabricated by sputtering the S/F/N/F/S multilayer onto a Si substrate, followed by subtractive patterning by photolithography and ion milling into circular junctions ranging in diameter from 10-80 microns. The critical current density of the junctions decays exponentially along the interfaces, and on HS and SHS systems through the half-metallic region takes place through a single conducting channel. Our calculations for these physically single mode setups single mode point contacts and chaotic quantum dots with single mode contacts illustrate the main strength of the scattering matrix approach: it allows for studying systems in the quantum mechanical limit, which is inaccessible for quasiclassical Green’s function methods, the main theoretical tool in previous works on the triplet proximity effect.

4:42PM L34.00011 Sign reversal of ac Josephson current in a ferromagnetic Josephson junction. SHIN-ICHI HIKINO, MICHIOYUKI MORI, SAUBERO TAKAHASHI, SATAMICHI MAEKAWA, Institute for Materials Research, Tohoku University — It is known that in a superconductor/insulator/superconductor (SIS) junction, when a finite voltage is applied, the Josephson current shows a logarithmic divergence, i.e., the so-called Riedel peak (RP) at the gap voltage, V=2Δ/ε (Δ is a superconducting gap). This result is observed in a double barrier Josephson junction such as SXS junction, on the other hand, the voltage dependence of Ic has not been investigated so far, where X is a normal metal (N) or a ferromagnet (F). We study the voltage dependence of Josephson critical current (Ic) in a variety of SXN junctions. In a SNS junction, Ic shows the RP at the gap voltage similar to a Josephson junction. In the SXS junction, Ic shows the RP at the gap voltage similar to a Josephson junction. On the other hand, in a SFS junction, Ic shows a damped oscillation with the alternation of sign as a function of thickness (d) of F due to π transition. The RP exhibits a strong dependence on d, and changes its sign. It is predicted that the RP disappears at the 0-π transition in the SFS junction.

4:54PM L34.00011 Sign reversal of ac Josephson current in a ferromagnetic Josephson junction. MAZIN A. KHASAWNEH, WILLIAM P. PRATT JR., NORMAN O. BURGE, Dept. of Physics and Astronomy, Michigan State University, East Lansing, MI 48824 — We have measured the critical current of Josephson junctions of the form Nb/Co/Ru/Co/Nb, where the two Co layers are exchange-coupled antiferromagnetically by the thin (0.6 nm) Ru interlayer. The antiferromagnetic coupling causes nearly complete cancellation of the intrinsic magnetic flux produced by the Co domains, and allows us to study large-area junctions with total Co thicknesses ranging from 2 to 20 nm — four times thicker than in previous studies of Nb/Co/Nb Josephson junctions [1]. The dependence of the critical current on an in-plane external magnetic field results in a nearly perfect Fraunhofer pattern, due to the intrinsic flux cancellation. The junctions were fabricated by sputtering the S/F/N/F/S multilayer onto a Si substrate, followed by substracted patterning by photolithography and ion milling into circular junctions ranging in diameter from 10-80 microns. The critical current density of the decays exponentially with Co thickness, with a characteristic decay length of λF = 2.2 nm. There is no sign of a crossover to a slower decay at large Co thicknesses, which, if observed, might be a signature of the predicted long-range spin triplet state [2]. [1] Robinson et al., Phys. Rev. Lett. 68, 177003, 2006. [2] Bergeret et al., Rev. Mod. Phys. 77, 1321, 2005. [Work Supported by US DOE under grant DE-FG02-06ER4634]

5:06PM L34.00012 Josephson junctions with a synthetic antiferromagnetic interlayer. MAZIN A. KHASAWNEH, WILLIAM P. PRATT JR., NORMAN O. BURGE, Dept. of Physics and Astronomy, Michigan State University, East Lansing, MI 48824 — We have measured the critical current of Josephson junctions of the form Nb/Co/Ru/Co/Nb, where the two Co layers are exchange-coupled antiferromagnetically by the thin (0.6 nm) Ru interlayer. The antiferromagnetic coupling causes nearly complete cancellation of the intrinsic magnetic flux produced by the Co domains, and allows us to study large-area junctions with total Co thicknesses ranging from 2 to 20 nm — four times thicker than in previous studies of Nb/Co/Nb Josephson junctions [1]. The dependence of the critical current on an in-plane external magnetic field results in a nearly perfect Fraunhofer pattern, due to the intrinsic flux cancellation. The junctions were fabricated by sputtering the S/F/N/F/S multilayer onto a Si substrate, followed by substracted patterning by photolithography and ion milling into circular junctions ranging in diameter from 10-80 microns. The critical current density of the decays exponentially with Co thickness, with a characteristic decay length of λF = 2.2 nm. There is no sign of a crossover to a slower decay at large Co thicknesses, which, if observed, might be a signature of the predicted long-range spin triplet state [2]. [1] Robinson et al., Phys. Rev. Lett. 68, 177003, 2006. [2] Bergeret et al., Rev. Mod. Phys. 77, 1321, 2005. [Work Supported by US DOE under grant DE-FG02-06ER4634]
were performed for dF functional local pseudopotential Hamiltonian and non equilibrium quantum transport calculations, MAIA G. DE-AC02-05CH11231. The computational resources were provided by the Reseau quebecois de calcul haute perfomance (RQCHP).

This discrepancy hasn't been understood yet. Up to now, only calculations using the local density approximation for the exchange-correlation functional (LDA) for the electron-phonon coupling calculated within density functional theory do not agree with measured values, in contrast to others phonon related properties.

Once functionalized metallic nanotubes can become insulators if sp transitions in S/F/S junctions. We find the characteristic length of oscillation (ξF) to be 7.9 ± 0.4 nm. Earlier studies [1] using a similar PdNi alloy in S/F/S junctions found ξF ≈ ξP ≈ 2.8 nm, however, those measurements were performed for δF between 4.5 and 14 nm. In our experiment, ξF1 > ξF2, indicating that our samples are in the regime E<sub>ex</sub>-τ > h [2, 3], where E<sub>ex</sub> is the exchange energy and τ is the mean free time between electron collisions in the ferromagnet. In spite of covering this wide range, we see no evidence of a crossover to a slower decay, which, if present, would be indicative of long-range spin triplet correlations [4].

This work is supported by US-DOE grant, DE-FG02-06ER46341.
3:30PM L35.00006 An LDA+$U$ study of the photoemission spectra of ground state phase of americium and curium1, 4:18PM L35.00004 An LDA+DMFT study of the photoemission spectra of ground state phase of americium and curium1

1The work is supported by the U. S. Dept. of Energy and the Welch Foundation.

3:42PM L35.00007 Tackling localized d-states: a systematic investigation by GW@LDA+$U$, HONG JIANG, RICARDO I. GOMEZ-ABAL, FHI, Berlin, Germany, PATRICK RINKÉ, UC Santa Barbara, USA; MATTHIAS SCHEFFLER, FHI, Berlin, Germany — First-principles modeling of systems with localized d-states is currently a great challenge in condensed matter physics. Density-functional theory (DFT) in the standard local-density approximation (LDA) proves to be problematic. This can be partly overcome by including local Hubbard $U$ corrections (LDA+$U$), but itinerant states are still treated on the LDA level. Many-body perturbation theory in the GW approach offers both a quasiparticle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for localized states), and is therefore promising for these systems. Here we present a systematic investigation of the $G_0W_0$ method based on LDA+$U$ ($G_0W_0$@LDA+$U$) for a series of prototype systems: 1) ZnS with semicore 3s-states, 2) ScN and TiO$_2$ with empty 3d-states and 3) late transition metal oxides (MnO, FeO, CoO and NiO) with partially occupied d-states. We show that for ZnS, ScN and TiO$_2$, the $G_0W_0$ band gap only weakly depends on $U$, but for the other transition metal oxides the dependence on $U$ is as strong as in LDA+$U$. These different trends can be understood in terms of changes in the hybridization and screening. Our work demonstrates that $G_0W_0$@LDA+$U$ withphysivalvalues of $U$ provides a balanced and accurate description of both localized and itinerant states.

3:54PM L35.00008 LDA+DMFT Charge Self-consistency Applied to Yb Valence Transition, ERIK YLVISAKER, WARNER PICKETT, UC Davis, ANDREW MCMAHAN, LNL, JAN KUNYES, University of Augsburg — Elemental ytterbium metal is known to undergo a gradual transition from a divalent spd$^0f^{14}$ state to a trivalent spd$^0f^{13}$ state in a pressure range of 0 to 34 GPa. We present LDA+DMFT studies of this transition, comparing three impurity solvers (Hirsch-Fye QMC, continuous time QMC and Hubbard I) with each other and with experimental data. All Yb states of interest are kept; no downfolding to a minimum basis is done. This implementation of DMFT (especially the QMC solvers) to the correlated f-orbitals gives reasonable agreement with the experimental transition. However, the neglect charge self-consistency is questionable for a valence transition where the concentration of valence electrons changes. Therefore we generalize the procedure and compare and contrast LDA+DMFT results with and without charge self-consistency for Yb using the Hubbard I impurity solver.

4:06PM L35.00009 Computation of phonon spectra from density-functional perturbation theory in the projector augmented-wave approach, MARC TORRENT, FRANCOIS JOLLET, CEA, DAM, DIF, F-91297 Arpajon, France, CHRISTOPHE AUDOUZE, Laboratoire Math. Appliquées, Ecole Centrale de Paris, Grande Voie des Vignes F-92295 Châtenay-Malabry, France, XAVIER GONZE, Unité PCPM, Université Catholique de Louvain. B-1348 Louvain-la-Neuve, Belgium — The density-functional perturbation theory expressions have been derived within the projector augmented-wave formalism (PAW) and compared to those found in the ultrasoft pseudopotential framework [1]. They have been recently implemented in the ABINIT package [2] in the case of perturbations of the atomic-displacement type. We summarize the key points of this implementation. The variational and non-variational forms of the 2nd-order total energy changes are detailed. The resolution of the variational principle by a generalized Sternheimer equation is explained (the 1st-order wave-function change is found with a band-by-band conjugate gradient algorithm). We focus on some difficulties: metallic electronic occupations, response to incommensurate perturbations of periodic systems... Results on pure compounds are presented; a comparison with results from pseudopotentials approach is performed in order to highlight the effect of the PAW methodology and its accuracy. [1] Audouze, Jollet, Torrent and Gonze. Phys. Rev. B 73, 235101 (2006); 78, 035105 (2008) [2] http://www.abinit.org.

4:18PM L35.00010 eliminating the V-representability problem via coarse-graining, PAUL LAMMERT, Pennsylvania State University — The mathematical foundations of density functional theory remain in an incomplete state, with old nagging problems and questions. I propose a coarse-grained approach to eliminating the V-representability problem and present results on differentiability of the Lie functional.

4:30PM L35.00011 Density Functional Theory and Semiclassical Methods1, PETER ELLIOTT, DONGHYUNG LEE, ATTILA CANGI, KIERON BURKE, University of California, Irvine — In this work we explore the relationship between semiclassical methods and density functional theory. There is a rich history between the two, for example, the gradient expansion approximation (GEA), on top of which DFT methods and density functional theory. There is a rich history between the two, for example, the gradient expansion approximation (GEA), on top of which all common generalized gradient approximations (GGAs) are built, may be derived semiclassically. However methods like Thomas-Fermi and the GEA miss important contributions from quantum oscillations, such as shell structure. In Ref. [1] we showed why these are missing and how, for a simple system, one could derive them. This led to approximations to the density and kinetic energy density which were non-local functionals of just the external potential. Interpreting these in the context of DFT, allows us to understand current approximations and improve them. In fact the potential scaling (re-)introduced in Ref. [1] can be used to derive new exact conditions on the universal functional of DFT and its components. This talk will discuss both the development of potential functionals and how they can be used to understand DFT.

1Supported by National Natural Science Foundation, China. Grant 10805029

4:42PM L35.00012 Correlation-Kinetic Contributions in the Mapping to Model Noninteracting Fermion and Boson Systems, XIAOYIN PAN2, Ningbo University, VIRAJT SAHNI, The Graduate Center CUNY — In the mapping from a system of electrons in an external field $\mathcal{F}_{\text{ext}} = -V v(r)$ to one of noninteracting fermions or bosons in their ground state with equivalent density $n(r)$, electron correlations due to the Pauli principle, Coulomb repulsion, and Correlation-Kinetic effects must be accounted for. Via Quantal Density Functional Theory (QDFT), it is proved that the contributions due to the Pauli principle and Coulomb repulsion to either mapping are the same. The application to atoms of the QDFT mapping to the model fermion system shows the corresponding Correlation-Kinetic energy contribution to be a very small fraction of the electron-interaction energy. In contrast, the same application of the QDFT mapping to the model boson system shows the corresponding Correlation-Kinetic energy to be a substantial fraction of the electron-interaction energy. Thus, whereas Correlation-Kinetic effects are insignificant in the mapping to the fermionic system, they play a significant role in the mapping to the model system of bosons.

1Quantum Density Functional Theory, Springer-Verlag, 2004

2Supported by National Natural Science Foundation, China. Grant 10805029
4:54PM L35.00013 DFT-MD simulations of shocked Xenon. RUDOLPH J. MAGYAR, THOMAS R. MATTSSON, Sandia National Laboratories — Xenon is not only a technologically important element used in laser technologies, jet propulsion and dental anesthesia, but it is also arguably the simplest material in which to study the metal-insulator transition at high pressure. Because of its closed shell electronic configuration, Xenon is often assumed to be chemically inert, interacting almost entirely through the van der Waals interaction, and at liquid density, is typically modeled well using Leonard–Jones potentials. However, such modeling has a limited range of validity as Xenon is known to form compounds at normal conditions and likely exhibits considerably more chemistry at higher densities when hybridization of occupied orbitals becomes significant. In this talk, we present DFT-MD simulations of shocked liquid Xenon with the goal of developing an improved equation of state. The relative importance of the van der Waals interaction compared to other Coulomb interactions is considered, and estimates of the relative accuracy of various density functionals are quantified. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

5:06PM L35.00014 Evaluation of Magnetic Moments using Bader Analysis. TOMOHARU SHIKAUCHI, KAZUO TSUMURAYA, Meiji University, Japan — Evaluation of the magnetic moments in solids is crucial in the computational physics. The moments have been calculated by an atomic sphere approximation or a Voronoi polyhedron approximation. There has been a method to partition the space with the minimum electron charge density surface, called zero flux planes, around each atom. The space is called Bader region. We apply the method to calculate the local magnetic moments of each atom depending on their circumstance using the first principle electronic structure calculation. We obtain the moments from the Bader charges using the up-spin charge and the down-spin charges. We apply the validity of this scheme to the analyses of the spin moments in Fe-N compounds, fcc Fe, and bcc Fe crystals and compare them with the experimental values. For Fe₃N, the difference of the moments between Fe(I) and Fe(II) atoms has been larger than that of the Voronoi method and is better agreement with the experimental values than the Voronoi method.

5:18PM L35.00015 Layered dilute magnetic semiconductors: A dynamical mean field study¹. MAJID NILI, UNJONG YU, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — We study ferromagnetism of layered dilute magnetic semiconductors within the Dynamical Mean Field Approximation. Our approach includes the spin-orbit coupling in the host compound and the interaction between the magnetic ions and the itinerant carriers using a modified double-exchange coupling. We simulate heterostructures with different distributions of magnetic ions: uniform doping, delta-doping in one single layer and delta-doping in two layers. We investigate the magnetic properties by changing the hole filling as well as the magnetic doping and the position of the doped layers in the heterostructure. We also include the on-site attraction potential between the magnetic ions and charge carriers to show its effect on the formation of the impurity band. We find that the ferromagnetic transition temperature and other properties strongly depend on the distribution of magnetic ions.

¹ This work was supported by the National Science Foundation through OISE-0730290, DMR-0548011, and DMR-0706379

Tuesday, March 17, 2009 2:30PM - 4:00PM –
Session L36 Panel Discussion: APS Publishing: Present and Future 408

2:30PM L36.00001 Panel Discussion: APS Publishing, Present and Future — This panel discussion will consist of a set of short presentations covering issues relevant to publication in the APS journals, including the concept of “significant” new physics, followed by questions and comments from the audience. The editors will comment on the identification of “significance” and its role in the editorial process, past, present, and future. There will be a brief “State of the Journals” address by APS Editor-in-Chief, Gene Sprouse, and statements of key issues facing the journals, by their editors. There will also be an introduction to the new APS publication Physics by its Editor, David Voss. The questions and comments section will be moderated by the Editor-in-Chief.

Tuesday, March 17, 2009 2:30PM - 5:06PM –
Session L37 DCP: Focus Session: Spectroscopic Probes of Biomolecular Structure and Function III 409

2:30PM L37.00001 UV Resonance Raman Discovery of Gibbs Free Energy Landscape for Protein Alpha Helix Folding. SANFORD ASHER, University of Pittsburgh — We developed a powerful method to follow the evolution of secondary structure in the amide peptide bonds of peptides and proteins. UV Raman excitation into these ~200 nm electronic transitions results in the enhancement of the amide vibrations of the peptide backbone. In our most recent studies we reassigned the amide III region and found a particular band (the amide III, band) which reports selectively on the Ramachandran Ψ angle and the state of peptide bond hydrogen bonding. We demonstrate that this band is Raman scattered independently by each peptide bond with insignificant coupling between peptide bonds. We also show that isotope editing of a peptide bond (by replacing the Cα–H with Cα–D) allows us to determine the frequency of an individual peptide bond within a peptide or protein which gives us its Ψ angle. Consideration of the Boltzmann equilibria allows us to determine the Ψ angle energy landscape which connects secondary structure conformations. The Ψ angle coordinate is the most important reaction coordinate required to enable the understanding of the mechanism(s) of protein folding.
3:42PM L37.0003 Inhibition of urinary calculi — a spectroscopic study¹ . FELICIA MANCIU, JAYESH GOVANI, WILLIAM DURRER, LAYRA REZA, LUIS PINALES, Physics Department, University of Texas at El Paso, El Paso, TX 79968 — We present multi-technique spectroscopic investigations by Raman, infrared absorption, X-ray photoelectron spectroscopy (XPS), and photoluminescence on the effects of the herb Rotula Aquatica Lour (RAL) on the growth of synthetically prepared Mg-based calculi of similar composition to common urinary calcui. Three samples were prepared; one MgPO₄-based standard and two others, separately incorporating 1 wt.% and 2 wt.% RAL herbal extract. Raman and infrared data show a newbeyrie structure for the crystals without and with inhibitor. XPS revealed the unexpected presence of Zn and a significant increase in Mg in the samples with RAL inhibitor. The presence of metallic Zn may contribute to the inhibition process by initiating rapid stone formation. XPS and Raman results also suggest another mechanism of inhibition by revealing evidence for Mg-O bonding between the plant extract and the phosphate units of urinary calculi. Similarity between our photoluminescence measurements and those of in vivo chlorophyll a provides additional evidence of Mg-related inhibition.

¹This work was supported by the NSF-MRI grant # 0723115. The authors are thankful to Dr. Mihir Joshi from Saurashtra University, Rajkot 360005, India, for providing the samples.

3:54PM L37.0004 Application of a Newly Built Chirped-Pulse Fourier Transform Microwave (CP-FTMW) Spectrometer to Study Biomolecules in the Gas Phase¹ . RYAN BIRD, DAVID PRATT, University of Pittsburgh, JUSTIN NEILL, BROOKS PATE, University of Virginia — Chirped-pulse Fourier Transform Microwave (CP-FTMW) spectroscopy is an exciting new technique that makes possible the recording of the complete microwave spectrum of a gas phase sample using a single 1 μs pulse. In this report, we will describe the recent introduction of a laser ablation nozzle for the study of small biomolecules using this technique.

¹Work supported by NSF (CHE-06 18740).

4:06PM L37.0005 Optical Conformational Transition Pathways of DsRed, Elucidated by Polarization-Modulated Fourier Imaging Correlation Spectroscopy . ANDREW MARCUS, ERIC SENNING, GEOFFREY LOTT, University of Oregon, MICHAEL FINK, Omega Optical, Inc — This work presents a novel ‘phase-selective’ approach to fluorescence fluctuation spectroscopy that simultaneously determines the joint probability distributions and two-dimensional spectral densities of protein conformational transitions, and nanometer center-of-mass displacements. Fourier imaging correlation spectroscopy (FICS) combines polarization- and intensity-modulated photo-excitation with phase-sensitive signal detection to monitor the collective coordinate fluctuations from a large population of fluorescent molecules (N ~ 10⁶). FICS is based on the principle that fluctuations of partially averaged molecular coordinates can be monitored through variations of an optical signal phase. Experiments are performed on DsRed, a tetrameric complex of fluorescent protein subunits, derived from a reef-building coral. Thermally induced conformational transitions of the DsRed complex lead to fluctuations in the optical dipolar coupling between adjacent chromophore sites. An analysis of polarization-resolved FICS fluctuation data, in terms of two-dimensional spectra and joint probability distributions, provides detailed information about cooperative ‘transition pathways’ between distinct dipole-coupled DsRed conformations.

4:18PM L37.0006 Insights on the Structural Details of Endonuclease EcoRI-DNA Complexes by Electron Spin Resonance . JESSICA SARVER, University of Pittsburgh — Pulsed electron spin resonance (ESR) was used to probe the binding specificity of EcoRI, a restriction endonuclease. Using site-directed spin labeling, a nitroxide side chain was incorporated into the protein, enabling the use of ESR to probe the structural details of EcoRI. Distance measurements were performed on EcoRI mutants when bound to varying sequences of DNA using the Double Electron-Electron Resonance experiment. These distances demonstrated that the average structure in the arm regions of EcoRI, thought to play a major role in binding specificity, is the same when the protein binds to different sequences of DNA. Also, it was determined that the arms exhibit higher flexibility when bound to sequences other than the specific sequence due to the larger distance distributions acquired from these spin labeled complexes. Molecular dynamics (MD) simulations were performed on the spin-label-modified specific EcoRI-DNA crystal structure to model the average nitroxide orientation. The distance distributions from MD were found to be narrower than experiment, indicating the need for a more rigorous sampling of the nitroxide conformers in silico.
4:30PM L37.00007 1D and 2D-IR spectroscopy of blended polymer-porphyrin thin films, AARON MASSARI, AUDREY EIGNER, PATRICK KONOLD, University of Minnesota, Twin Cities — One and two-dimensional IR spectroscopies are used to study the static and dynamic environments that form when ruthenium(tetraphenyl)porphyrin carbonyl is blended with regioregular poly(3-hexylthiophene). The 1D-IR spectra of the Ru-bound CO symmetric stretch indicate the development of several inhomogeneously broadened microenvironments as the concentration of porphyrin is increased. Transmission electron microscopy is used to characterize the blended films, which show evidence of phase-segregation. By correlating the degree of separation with the relative proportions of each component of the 1D-IR spectrum, we identify the IR spectra corresponding to the free and aggregated porphyrin-CO stretches. 2D-IR vibrational echo spectroscopy is then used to measure the ultrafast dynamics that are present in the polymer and porphyrin phases.

4:42PM L37.00008 Microtubule-associated-protein (MAP) Tau Regulates the Number of Protofilaments in Microtubules: A Synchrotron X-ray Scattering Study, MYUNG CHUL CHOI, UCSD, URI RAVIV, Univ. Jerusalem Israel, HERBERT MILLER, MICHELLE GAYLORD, ERKAN KIRIS, DONOVAN VENTIMIGLIA, UCSD, DANIEL NEEDLEMAN, Harvard Univ., MAHN WON KIM, KAIST, LESLIE WILSON, STUART FEINSTEIN, CYRUS SAFINYA, UCSD — Microtubules (MTs), 25 nm protein nanotubes, are a major filamentous element of the cytoskeleton involved in intracellular trafficking and cell division. MAP tau regulates tubulin assembly and MT stability. Dysfunction of tau has been correlated with numerous neurodegenerative diseases. We describe our recent findings about the effects of six naturally occurring central nervous system (CNS) tau isoforms on the assembly structure of taxol-stabilized MTs, using synchrotron small angle x-ray scattering (SAXS). Most significantly, we found that tau, at low binding density, regulates the distribution of protofilament numbers in MTs. DOE DE-FG02-06ER46314, NSF DMR-0803103, NIH RO1-NS35010 and NS13560.

Tuesday, March 17, 2009 2:30PM - 5:30PM — Session L38 DCP: Focus Session: Theory of Electron Transport Through Molecules III

2:30PM L38.00001 Statistical mechanics of non-equilibrium steady state systems, DANIEL KOSOV, University of Maryland — One of the important classes of non-equilibrium systems is the systems, which are maintained in non-equilibrium steady state by the contact with several external macroscopic reservoirs. These systems are ubiquitous and their theoretical description has been a challenging fundamental scientific problem for many years. They are also of significant practical interest for various nanotechnological and biological applications, such as quantum contacts, molecular motors, nanowires, and molecular junctions. There is no unique theoretical approach to wide variety of non-equilibrium steady state systems. General theoretical description of non-equilibrium steady states has not been developed yet and many fundamental theoretical questions are yet to be answered. For example, how to include many-particle correlation effects into theoretical treatment, is there exist a general variational principle for non-equilibrium steady state, do we enforce by the choice of a particular theoretical treatment a specific non-equilibrium steady state which is not the same as the real system would establish under the same boundary conditions, do we have a unique steady state in a system of non-equilibrium interacting particles for given boundary conditions? In my talk, I will review these questions and their relevance to electron transport through molecules. I will also give account of our recent computational and theoretical work on non-equilibrium quantum transport through molecular nanostructures.

3:06PM L38.00002 Vibronic effects in single molecule conductance1, MICHAEL THOSS, Department of Chemistry, Technical University of Munich — Recent experimental advances have allowed to study the conductance properties of single-molecule junctions and revealed a wealth of intriguing transport phenomena. An important aspect that distinguishes nanoscale molecular conductors from mesoscopic devices is the influence of the nuclear degrees of freedom of the molecular bridge. Due to the small size of molecules, the charging of the molecular bridge is often accompanied by significant changes of the nuclear geometry that indicate strong coupling between electronic and nuclear (in particular vibrational) degrees of freedom. In this contribution, the effect of electron-vibrational (vibronic) coupling on the transport properties of single molecule junctions is studied. The study is based on a combination of first-principles electronic structure calculations to characterize the system and different transport methods including inelastic scattering theory, master equations and nonequilibrium Green's function theory. The basic mechanisms of vibrationally coupled electron transport are analyzed for a generic model of a molecular junction as well as benzenealkanethiolates between gold electrodes. The results show that vibronic coupling can have a significant effect on the conductance of molecular junctions. It manifests itself in pronounced structures in the current-voltage characteristics. Moreover, the current-induced excitation of vibrational modes may result in a significant deviation of the vibrational degrees of freedom from their equilibrium distribution.

3:42PM L38.00003 Controlling Current Flow Through Molecules With Electric Fields Emerging From Nearby Molecules: Theory and Experiment2, G. KIRCZENOW, Simon Fraser U., P. G. PIVA, R. A. WOLKOW, NINT and U. of Alberta — We show that electrical conduction through molecules can be strongly modulated by electric fields of nearby polar molecules. We study 1D organic heterostructures consisting of contiguous lines of CF3-styrene and OCH3-styrene molecules on H-terminated Si(100). For suitable alignment of the OCH3 groups in the molecular chain, their combined electric fields are shown by density functional calculations to give rise to potential profiles along the OCH3-styrene chain that result in strongly enhanced conduction transverse to the CF3-styrene/OCH3-styrene heterojunction for moderately low negative substrate bias, as is observed by STM. Under similar bias, dipoles associated with CF3 groups are found in both theory and experiment to depress transport in the underlying Si. Under positive substrate bias, simulations suggest that the structural and electrostatic properties of CF3-styrene molecules may lead to more sharply localized conduction enhancement near the heterojunction. Thus choice of substituents, their attachment site on the host styrene molecules on Si and the orientations of the molecular dipoles and multipoles provide a means of differentially tuning transport on the molecular scale.

1Supported by CIFAR, NSERC, iCORE, Westgrid, NRC and INMS

2Supported by CIFAR, NSERC, iCORE, Westgrid, NRC and INMS
3:54PM L38.00004 Effects of Dephasing on DNA Sequencing via Transverse Electronic Transport1, MATT KREMS, University of California, San Diego, YURIY PEPSHIN, University of South Carolina, MICHAEL ZWOLAK, Los Alamos National Laboratory, MASSIMILIANO DI VENTRA, University of California, San Diego — We study theoretically the effects of dephasing on DNA sequencing in a nanopore via transverse electronic transport. To do this, we couple classical molecular dynamics simulations with transport calculations using scattering theory. Previous studies, which did not include dephasing, have shown that by measuring the transverse current of a particular base multiple times, one can get distributions of currents for each base that are distinguishable. We introduce a dephasing parameter into transport calculations to simulate the effects of the ions and other fluctuations which are not included in the Landauer approach. We find that the overall dephasing required for good contact transparency is broken by connecting through a six-member ring on the tube. Full dephasing is achieved by an all-carbon contact through a five-member ring leads to near perfect contact transparency for different conjugated molecular bridges. [Phys. Rev. Lett. 99, 146802 (2007)]

4:06PM L38.00005 Single-Electron Transistors made by chemical patterning of silicon dioxide substrates and selective deposition of gold nanoparticles. ULAS COSKUN, HENOK MEABRANTU, Physics Department Duke University, THOM LABEAN, Chemistry Department, Duke University, GLEB FINKELSTEIN, Physics Department Duke University — We describe a method to pattern SiO2 surfaces with colloidal gold nanoparticles by e-beam lithography and selective nanoparticle deposition. The method allows us to deposit nanoparticles in different shapes, including long continuous lines just one nanoparticle wide. We contact the pre-positioned nanoparticles with metal leads to form Single Electron Transistors. The Coulomb blockade pattern surprisingly does not show the parasitic “offset charges” at low temperatures, indicating relatively little surface contamination.

4:18PM L38.00006 Contact Transparency of Nanotube-Molecule-Nanotube Junctions, S. H. KE, H. U. BARANGER, WENTAO YANG, Duke University — The transparency of contacts between conjugated molecules and metallic single-walled carbon nanotubes is investigated using a single-particle Green’s function method which combines a Landauer approach with ab initio density functional theory. We find that the overall dephasing required for good contact transparency is broken by connecting through a six-member ring on the tube. Full dephasing is achieved by an all-carbon contact through a five-member ring leads to near perfect contact transparency for different conjugated molecular bridges. [Phys. Rev. Lett. 99, 146802 (2007)]

4:30PM L38.00007 Quantum many-body effects on the electric and thermoelectric response of molecular heterojunctions, JUSTIN BERGFIELD, CHARLES STAFFORD, University of Arizona — A semi-empirical e-electron Hamiltonian (extended Hubbard model) is used to model the electronic degrees of freedom most relevant for transport in a heterojunction consisting of a conjugated organic molecule coupled to two (or more) metallic electrodes. With an appropriate choice of parameters, the complete spectrum of electronic excitations of the molecule up to 8–10eV can be accurately described, which is essential to accurately model transport far from equilibrium. The electric and thermoelectric response of the junction is calculated within a many-body theory of transport based on nonequilibrium Green’s functions. For benzenedithiol-Au junctions, the parameters characterizing the lead-molecule coupling (tunneling width and chemical potential offset) are determined by comparison to linear-response measurements of conductance and thermopower. The nonlinear transport can then be predicted: the differential conductance as a function of gate and bias voltages exhibits clear signatures of charge quantization and resonant tunneling through excited states, with an irregular “molecular diamond” structure analogous to the regular Coulomb diamonds observed in quantum dot transport experiments. Several other small conjugated organic molecules are also investigated. [C. W. M. Castelon and W. Barford, J. Chem. Phys. 117, 3570 (2002)].

4:42PM L38.00008 Current induced local heating and heat transport in single molecular bridge junction, YOSHIHIRO ASAI, AIST, Umesono 1-1-1, Central 2, Tsukuba, Ibaraki 305-8568, Japan — Current induced local heating will be discussed theoretically. Both electronic and thermal conductance of electronic and phonon conduction are calculated in a microscopic way, including inelastic scattering effects due to electron-phonon coupling. [1] Based on the self-consistent solution of an alkanedithiol molecule bridging gold electrodes, we found that the effective temperature $T_{eff}$ due to the local heating is largely reduced by the heat conductance, which releases the Joule heat out of the molecule. All these calculations are made in a fully microscopic way without introduction of the phenomenological phonon diffusion effect used in literature. Theoretical voltage dependence of $T_{eff}$ agrees nicely with an experiment. [2 Ref.] [1] Y. Asai, Phys. Rev. B78, 045434 (2008). [2] Z.Huang et al, Nano Letters, 6, 1240 (2006).

5:06PM L38.00009 Fabrication and characterization of vertically aligned and interconnected nickel oxide Nanowalls1, LATHA KUMARI, WENZHI LI, Florida International University, CHARLES H. VANNOY, ROGER M. LEBLANC, University of Miami, DEZHI WANG, Boston College, DEPARTMENT OF PHYSICS, FLORIDA INTERNATIONAL UNIVERSITY, MIAMI, FL 33199, USA TEAM, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MIAMI, CORAL GABLES, FL 33124, USA COLLABORATION, DEPARTMENT OF PHYSICS, BOSTON COLLEGE, CHESTNUT HILL, MA 02467, USA COLLABORATION — Vertically aligned and well interconnected NiO nanowalls were fabricated on Ni foil by a two step hydrothermal route. The as-prepared nickel hydroxide was converted to NiO by further heat treatment. The NiO nanowalls are typically 15 nm thick and around 1-1.5 µm wide. The NiO nanowalls have cubic crystal structure with their growth plane along the [111] direction. The NiO nanowalls show an optical band gap of about 3.8 eV and exhibit broad photoluminescence emission band centered at around 390 nm. The present synthesis technique allows the growth of well aligned 2D nanostructures with large surface area for possible applications in nanoscale devices.

1W.Z. Li acknowledges the support by National Science Foundation under grant DMR-0548061.

5:18PM L38.00011 ABSTRACT WITHDRAWN
2:30PM L39.00001 Biochemistry on a leash: Confinement as a regulatory mechanism for bimolecular reaction rates, DANIEL REEVES, KEITH CHEVERALLS, JANE KONDEV, Brandeis University — We describe two mechanisms by which confinement regulates diffusion-limited bimolecular reaction rates. The first mechanism, illustrated by the actin capping protein formin, uses a flexible polymer to tether ligand binding sites, which serve as intermediaries, to the reactive site. The second mechanism uses a potential (e.g. hard wall potential), to constrain the motion of a ligand receptor within a confining volume. We analyze both mechanisms theoretically, using a combination of analytic and numerical techniques, to obtain the steady state binding kinetics. We explore how the reaction rates are regulated by parameters of the model such as the length of the polymer tether, and use our findings to explain the key features of the formin system. Finally, we suggest other systems, both synthetic and biological, in which these mechanisms for regulating bimolecular reactions might be at play.

2:42PM L39.00002 Crowded, cell-like environment induces shape changes in aspherical protein, MARGARET CHEUNG, University of Houston — How the crowded environment inside cells affects the structures of proteins with aspherical shapes is a vital question because many proteins and protein–protein complexes in vivo adopt anisotropic shapes. Here we address this question by combining computational and experimental studies of a football-shaped protein (i.e. *Borreia burgdorferi* VlsE) under crowded, cell-like conditions. The results show that macromolecular crowding affects protein-folding dynamics as well as overall protein shape. In crowded milieus, distinct conformational changes in VlsE are accompanied by secondary structure alterations that lead to exposure of a hidden antigenic region. Our work demonstrates the malleability of “native” proteins and implies that crowding-induced shape changes may be important for protein function and malfunction in vivo.

3:18PM L39.00003 Molecular dynamics study of multimerization of the Mms6 protein from Magnetospirillum magnetism strain AMB-1, MONICA LAMM, RASTKO SKNEPNEK, LIJUN WANG, MARIT NILSEN-HAMILTON, Iowa State University and Ames Laboratory — In order to optimize their search for nutrients, magnetotactic bacteria have developed an ability to align themselves to Earth’s magnetic field. This is achieved by forming a chain of vesicles containing magnetite superparamagnetic nanoparticles with sizes of the order of 50nm. The presence of the small protein Mms6 plays an important role in the successful in vitro growth of magnetite nanoparticles, although the mechanism of this process is not understood. Preliminary experiments on Mms6 in solution indicate that the protein forms multimers of variable sizes, depending on the salt concentration. Using an intermediate level coarse grained model for Mms6 we investigated the formation of these multimers as a function of temperature and salt concentration.

3:30PM L39.00004 The Packing of Flexible Screws and the Self-Limited Assembly of Biopolymer Bundles, GREGORY GRASON, University of Massachusetts, Amherst — Living cells rely heavily on assemblies of filamentous proteins, such as F-actin and microtubules, to perform a variety of tasks, ranging from adhesion and locomotion to cell division and intracellular transport. In the dynamic cellular environment, the efficiency of these tasks is crucially dependent on the robust assembly and disassembly of rope-like bundles of filamentous molecules. Recent in vitro studies of F-actin assembly [Lai et al., Phys. Rev. Lett. (2007)] suggest that bundle formation may take place as an equilibrium process, with a thermodynamically-preferred bundle diameter. Within the context of a generalized elastic model of filament packings, we explore the possibility that limited-bundle growth is directly linked with the intrinsic chiral structure of biological filaments themselves. The hexagonal packing of biopolymers leads to the build up of chiral stress, or torque, that generically induces the formation of twisting filament bundles of finite size. We demonstrate that the underlying elasticity of the bundle—i.e. whether hexagonal-solid or hexagonal-columnar—plays a key role in dictating both the thermodynamics (i.e. disperse, bundled or bulk aggregation) and structure (i.e. size and twist) of “self-braiding” aggregates of helical filaments.

4:06PM L39.00005 Simulation of signal transduction in model multiprotein systems, JULIUS SU, Caltech — To simulate the dynamics of multiprotein machines, I have developed a method called multiconformer Brownian dynamics (mcBD). In this method, proteins rotate and translate via Brownian motion while their conformations are varied among a prestored set of structures on a simplified energy landscape. As an example, I build a simple model of a G-protein coupled receptor/G-protein complex, and show that ligand binding causes conformational shifts, which induce GDP to leave, GTP to bind, and the complex to dissociate. The two proteins couple their fast rotations and translations via Brownian motion while their conformations are varied among a prestored set of structures on a simplified energy landscape.

4:18PM L39.00006 Implicit solvent model for linear-scaling first-principles electronic structure calculations, HATEM H. HELAL, MIKE PAYNE, Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, ARASH A. MOSTOFI, Departments of Physics and Materials, Imperial College London — Density functional theory (DFT) enables first-principles calculations that exhibit cubic scaling of the computational time required with respect to the number of atoms in the system. This presents an unavoidable difficulty when first-principles accuracy is needed for the study of large-scale biological systems. The ONETEP program reformulates DFT so that the required computational effort scales only linearly with system size, recently demonstrated for up to 32,000 atoms on 64 cores. Further complicating DFT based studies of biomolecular systems is the need for an accurate representation of the electrostatic environment. Rather than introducing explicit solvent molecules into the system, which would be computationally prohibitive, we present our recent efforts to integrate an implicit solvent model with ONETEP in order to study systems in solution consisting of many thousands of atoms. We report preliminary results of our methodology with a study of the DNA nucleosome core particle.

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4:30PM L39.00007 Using stochastic dynamics to validate runtimes of protein simulations1

STEPHEN D. HICKS, CHRISTOPHER L. HENLEY, Cornell University — We use short molecular dynamics simulations (~200 cpu-hr, using NAMD) of individual bonds between capsid proteins to microscopically determine coarse-grained elastic parameters of entire virus capsids. In particular, we treat each protein (or for larger proteins, each domain) as a rigid body described by a 6-vector of translational and orientational degrees of freedom, $\dot{\mathbf{x}}(t)$. We then model the evolution of the relative positions as an overdamped random walk, $\mathbf{x}(t) = -K_{ij} \dot{\mathbf{x}}(t) + \zeta(t)$, where $\zeta(t)$ are random variables satisfying $\langle \zeta(t) \rangle = 0$. Our goal is to determine the stiffness matrix $K_{ij}$, but this requires long-time data to measure accurately. We therefore measure the noise matrix $2\Gamma_{ij}$, which depends on much shorter timescales, and compute the relaxation times by diagonalizing $\Gamma = T \Delta \Gamma T$. Although we use biologically relevant configurations in each simulation, we have taken the domains out of their full context by simulating one pair at a time, and therefore external stresses are missing, which we measure from the drift and compensate for in subsequent simulations. Finally, we apply this technique to the HIV capsid protein.

1Supported by DOE grant DE-FG02-89ER-45405

4:42PM L39.00008 A symplectic integration method for elastic filaments

TAYLOR LADD, GAURAV MIRSA, University of Florida — Elastic rods are a ubiquitous coarse-grained model of semi-flexible biopolymers such as DNA, actin, and microtubules. The Worm-Like Chain (WLC) is the standard numerical model for semi-flexible polymers, but it is only a linearized approximation to the dynamics of an elastic rod, valid for small deflections; typically the torsional motion is neglected as well. In the standard finite-difference and finite-element formulations of an elastic rod, the continuum equations of motion are discretized in space and time, but it is then difficult to ensure that the Hamiltonian structure of the exact equations is preserved. Here we discretize the Hamiltonian itself, expressed as a line integral over the contour of the filament. This discrete representation of the continuum filament can then be integrated by one of the explicit symplectic integrators frequently used in molecular dynamics. The model systematically approximates the continuum partial differential equations, but has the same level of computational complexity as molecular dynamics and is constraint free. Numerical tests show that the algorithm is much more stable than a finite-difference formulation and can be used for high aspect ratio filaments, such as actin. We present numerical results for the deterministic and stochastic motion of single filaments.

5:06PM L39.00009 Biomolecular Structure Determination with Divide and Concur

YOAV KALLUS, VEIT ELSER, Cornell University — Divide and concur $D - C$ is a general computational approach, designed for the solution of highly frustrated problems. Recently applied to the problems of disk packing, the kissing number problem, and 3-SAT, it was competitive or outperformed special-purpose methods. We present a new method, adaptive anisotropic network model (aANM) for exploring functional transitions, based on the elastic network models which have been widely used to describe the collective dynamics of biomolecular systems. Application to bacterial chaperonin GroEL highlights the utility of the methodology. Comparisons with experimental data and results from action minimization algorithm support the utility of aANM as a computationally efficient, yet physically plausible, tool for unraveling potential transition pathways sampled by large complexes/ensembles and assessing the critical inter-structures formed/broken near the transition state(s), most of which involve conserved residues.

5:18PM L39.00011 Generic Coarse-Grained Model for Protein Folding and Aggregation

TRISTAN BEREAU, MARKUS DESERNO, Dept. of Physics, Carnegie Mellon University, Pittsburgh, PA 15213 — The complexity involved in protein structure is not only due to the rich variety of amino acids, but also the inherent weak interactions, comparable to thermal energy, and important cooperative phenomena. This presents a challenge in creating a unified model that captures the diversity of the sequence space. We developed a model that captures the diversity of the sequence space by using a coarse-grained approach. We tested our model on a variety of proteins and found that it accurately predicts the stability of the native state. We also found that the model is able to predict the aggregation of proteins, which is a key factor in the formation of amyloids.

5:30PM L39.00012 Computational Investigation of Conformational Changes in Proteins upon Adsorption

SUMIT SHARMA, Columbia University, GAURAV ANAND, GEORGES BELFORT, Rensselaer Polytechnic Institute, SANAT K. KUMAR, Columbia University — Amyloidogenic diseases, such as, Alzheimer’s, are caused by adsorption and aggregation of partially unfolded proteins. Protein adsorption is often accompanied by conformational rearrangements, which are thought to affect many properties such as their adhesion strength to the surface, biological activity, and aggregation tendency. Experiments have shown that many proteins, upon adsorption to hydrophobic surfaces, undergo a helix to sheet or random coil secondary structural rearrangement. To better understand the equilibrium structural complexities of this phenomenon, we have performed Monte Carlo (MC) simulations and Single Chain Mean Field calculations of adsorption of different proteins, modeled as lattice chains, to study the adsorption behavior and equilibrium protein conformations at different temperatures, protein concentration and surface hydrophobicity. Free energy and entropic effects on adsorption have been studied by determining density states using Weighted Histogram Analysis Method. Conformational transitions of proteins on surfaces will be discussed as a function of surface hydrophobicity.

5:42PM L39.00013 Role of van der Waals interactions for the intrinsic stability of polyalanine helices

ALEXANDRE TKATCHENKO, VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, Germany, JOEL IRETA, Dep. Quimica, UAM-Iztapalapa, Mexico, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — The helical motif is an ubiquitous conformation adopted by amino acid residues in a protein structure and helix formation is the simplest example of the protein folding process. How stable is the folded peptide helix in comparison to a random coil structure? What are the interactions responsible for stabilizing the helical conformation? Answering these questions has thus a direct implication for understanding protein folding. In this work we use density functional theory (DFT) augmented with a non-empirical correction for van der Waals (vdW) forces to study the stability of alanine polypeptide helices in vacuo. We find a large stabilization of the native helical forms when vdW correction is used. It amounts to 121%, 157% and 83% on top of the Perdew-Burke-Ernzerhof (PBE) functional in the case of infinite $\alpha$, $\beta$ and $\pi$ helices, respectively. Thus, the experimentally observed $\alpha$ helix is significantly stabilized by vdW forces both over the fully extended and the $3_{10}$ conformations. Our findings also suggest an explanation to the remarkable stability of gas-phase alanine helices up to high temperatures [M. Kohtani et al. JACS 126, 7420 (2004)].
2:42PM L40.00002 Density fluctuations in confined and non-confined DNA

JUNHAN PAN, CHUNDA ZHOU, ROBERT RIEHN, North Carolina State University — DNA stretching in quasi one-dimensional nanochannels is an emerging technique for the analysis of genomic-sized DNA molecules. For formulating an optimal measurement strategy, the thermal fluctuations of confined molecules are of crucial importance. While previous measurements have concentrated only on the end-to-end length, we present here an experimental study of density fluctuations within the molecule, and find a good agreement with a model similar to a oscillator chain. We further discuss how such a model leads to a natural interpretation of the interesting intramolecular collapse of DNA that we recently under application of a.c. electric fields at frequencies of a few hundred Hertz.

2:54PM L40.00003 Direct Observation of Multiple Pathways of DNA Stacking Using Single-Molecule AFM

CHING-HWA KIANG, WEI-HUNG CHEN, Department of Physics and Astronomy, Rice University, Houston, TX 77005 — During DNA interactions, single-stranded DNA (ssDNA) is often stretched and stabilized by coupling with ssDNA binding proteins to serve as an intermediate state. The conformational and energetic changes of stretched DNA are of great interest because of their relevance in biological functions. Direct manipulation of DNA has yielded much of the information about the mechanical properties of DNA without the complication of interacting molecules. Stretching ssDNA has provided direct measurement of the base stacking mechanics and energetics. For example, polyA has been shown to have two transitions during overstretching. Here we showed direct observation of two overstretching pathways during the second transition. We have observed “hopping” between these two pathways during constant-force measurements. We will discuss the implications of such transition and its significance in biological functions.

3:06PM L40.00004 Stabilities of Constituent Hairpins Determine Whether RNA Folds via Ordered and/or Parallel Mechanisms

SAMUEL CHO, DEVARAJAN THIRUMALAI, University of Maryland — RNA molecules are increasing becoming seen as a set of critical players in numerous cellular processes, and a firm understanding of their folding energy landscapes is essential for understanding how they carry out their functions. While it might seem natural to assume that the simplicity of RNA molecules, with only four possible bases, dictate that they must fold via simple mechanisms, experiments continue to point to complex folding energy landscapes involving parallel mechanisms. In our present study, we address how even simple RNA molecules can give rise to very complex folding mechanisms. We begin by making the argument that the complexity observed for RNA folding are in fact fully expected because the lack of variability of the RNA subunits leads to a lack of specificity for folding to the native basin. To illustrate our point, we performed coarse-grained simulations of three RNA pseudoknots and a tRNA molecule, which each are all relatively simple RNA molecules that contain at least two hairpins. From our simulations, we find that the main determinant for how these RNA molecules fold is largely dependent on the relative stabilities of their constituent hairpins. Ordered mechanisms arise if the stabilities of the constituent hairpins are sufficiently dissimilar and parallel folding mechanisms occur if the stabilities of the hairpins are similar.

3:18PM L40.00005 Structural basis of pathway-dependent force profiles in DNA

DANIEL ROE, ANNE CHAKA, Physics Laboratory, National Institute of Standards and Technology — Since DNA must bend and/or stretch to perform many of its functions, it is important to understand the mechanical properties of DNA. Single molecule experiments have been able to study the response of DNA to applied forces. One interesting result of such studies is that at high loading rates a greater force is required to stretch DNA when pulling from the 3' ends as opposed to the 5' ends. While these experiments provide valuable insights into the stability of DNA, it is often difficult to relate the results to specific structural changes. We have used molecular dynamics simulation methods to study the structure and dynamics of DNA under a tensile load. Simulations were performed on a variety of fully solvated DNA sequences up to 30 base-pairs in length, and were conducted under both non-equilibrium and equilibrium conditions. Different stretched DNA structures are observed depending on whether pulling occurs from the 5' ends or 3' ends. Detailed analysis of these structures provides a direct structural explanation of the observed difference between 3' and 5' pulling.

3:30PM L40.00006 Folding Kinetics of Riboswitch Transcriptional Terminators

BENJAMIN SAUERWINE, MICHAEL WIDOM, Carnegie-Mellon University — Riboswitches control the expression of genes in bacteria by halting gene transcription or allowing it to proceed based on the presence of ligands in solution. A key feature of every riboswitch is a transcriptional terminator in which the messenger RNA folds into a secondary structure with the stem-loop structure of a hairpin. Through kinetic Monte Carlo simulation we show that terminators have been naturally selected to fold with high reliability on the time-scale of gene transcription. This efficient folding behavior is preserved among two classes of riboswitch and among two species of bacteria.

3:42PM L40.00007 First Principles Study of Nuclear Quadrupole Interactions in Single and Double Chain DNA and Solid Nucleobases

T.P. DAS, R.H. PINK, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, H.P. SAHA, LEE CHOW, UCF Orlando, M.B. HUANG, SUNY Albany — Nuclear Quadrupole Interactions (NQI) of \(^{17}O, ^{14}N\) and \(^{2}H\) nuclei have been studied for free nucleobases and nucleobases in single strand and double strand DNA and in solid state. Our first-principles investigations were carried out using the Gaussian 2003 set of programs to implement the Hartree-Fock procedure combined with many-body effects including using many-body perturbation theory. As expected for NQI in general, many-body effects are found to be small. Results will be presented for the quadrupole coupling constants \((e^2qQ)\) and asymmetry parameters \((\eta)\) for the nucleobases in various environments. Trends in \(e^2qQ\) and \(\eta\) in the different environments will be discussed. In the case of the solid nucleobases, comparisons will be made with available experimental data [1] for \(^{17}O\) nuclei.

3:54PM L40.00008 Optical control of DNA radio-sensitivity, RAMIN ABOLFATH, University of Texas, Southwestern Medical Center, Dallas — We explore the manipulation of the radio-sensitivity of the DNA molecules driven by the spin blockade mechanism of diffusive free radicals. We propose a mechanism which uses the simultaneous application of circularly polarized light and an external magnetic field to control the polarization of the free radicals and create an $S = 1$ electron-hole spin excitation (exciton) on DNA molecules. It allows us to manipulate and partially suppress the damage induced by ionizing radiation. We deploy an ab-initio molecular dynamics model to calculate the characteristic parameters of the light needed for optical transitions and investigate the effect of spin-injection on the formation of a free energy barrier in diffusion controlled chemical reaction pathways that controls radiation-induced DNA damage. As a specific example, we present the numerical results calculated for a nucleotide-base, e.g., Guanine, in the presence of an OH free radical.

4:06PM L40.00009 Acetylated histone H3 increases nucleosome dissociation1, MAREK SIMON, Department of Physics, The Ohio State University, MRIDULA MANOHAR, JENNIFER OTTESEN, Department of Biochemistry, The Ohio State University, MICHAEL POIRIER, Department of Physics, The Ohio State University — Chromatin’s basic unit structure is the nucleosome, i.e.: genomic DNA wrapped around a particular class of proteins – histones – which due to their physical hindrance, block vital biological processes, such as DNA repair, DNA replication, and RNA transcription. Histone post-translational modifications, which are known to exist in vivo, are hypothesized to regulate these biological processes by directly altering DNA-histone interactions and thus nucleosome structure and stability. Using magnetic tweezers technique we studied the acetylation of histone H3 in the dyad region, i.e. at K115 and K122, on reconstituted arrays of nucleosomes under constant external force. Based on the measured increase in the probability of dissociation of modified nucleosomes, we infer that this double modification could facilitate histone chaperone mediated nucleosome disassembly in vivo.

1This work was supported by a Career Award in the Basic Biomedical Sciences from the Burroughs Wellcome and NIH grant No. R01 GM083055.

4:18PM L40.00010 First Principles Study of Muonium Trapping and Associated Magnetic Hyperfine Interactions in Nucleobases in Single and Double Chain DNA and Solid Nucleobases, S.R. BADU, R.H. PINK, SUNY Albany, ARCHANA DUBAY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, H.P. SAHA, UCF Orlando, K. NAGAMINE, UC Riverside, E. TORIKAI, Yamanashi University, LEE CHOW, UCF Orlando, M.B. HUANG, T.P. DAS, SUNY Albany — The trapping of muonium (Mu) and muon hyperfine interactions (HFI) are studied for free nucleobases and nucleobases in single and double strand DNA and in solid nucleobases. For our investigations we have utilized the Hartree-Fock procedure with many-body effects included using many-body perturbation theory. Results for the muon magnetic contact and dipolar HFI will be presented for the various environments. The trends among the different environments is rather different from those for the nuclear quadrupole interactions in the corresponding systems because of the differences in geometry of the Mu trapping sites in the various systems. Quantitative comparison will be made between our theoretical results and experimentally measured$[^1]$muon HFI properties in the solid nucleobases.


4:30PM L40.00011 Modeling nucleic acid structure in the presence of single-stranded binding proteins1, ROBERT FORTIES, RALF BUNDSCUH, The Ohio State University — There are many important proteins which bind single-stranded nucleic acids, such as the nucleocapsid protein in HIV, the RecA DNA repair protein in bacteria, and all proteins involved in mRNA splicing and translation. We extend the Vienna Package for quantitatively modeling the secondary structure of nucleic acids to include proteins which bind to unpaired portions of the nucleic acid. All parameters needed to model nucleic acid secondary structures in the absence of proteins have been previously measured. This leaves the footprint and sequence dependent binding affinity of the protein as adjustable parameters of our model. Using this model we are able to predict the probability of the protein binding at any position in the nucleic acid sequence, the impact of the protein on nucleic acid base pairing, the end-to-end distance distribution for the nucleic acids, such as the nucleocapsid protein in HIV, the RecA DNA repair protein in bacteria, and all proteins involved in mRNA splicing and translation. We extend persistence length to dynamics on larger scales. [1] arXiv:0809.0667v1, Macromolecules in press (2008).

4:42PM L40.00012 A theoretical investigation of the interconversion between B and Z-DNA using the Adaptively Biased and Steered Molecular Dynamics methods, MAHMOUD MORADI, CHISTOPHER ROLAND, VOLODYMIR BABIN, CELESTE SAGUI, CHIPS and Department of Physics, North Carolina State University — The transition between right-handed B-DNA and left-handed Z-DNA in an implicit solvent environment was investigated via the free energy landscape of DNA as a function of the collective variables of handedness and radius of gyration, using the recently developed Adaptively Biased Molecular Dynamics (ABMD) method. The ABMD method, which belongs to the general category of umbrella sampling methods with a time-dependent potential, allows for an efficient and accurate estimation of the free energy barriers associated with the transition, especially when combined with multiple-walker and umbrella correction runs. The ABMD results are compared to those obtained using the Steered Molecular Dynamics (SMD) method. The implication of all these free energy results on the microscopics of the B to Z-DNA transition is to be discussed.

4:54PM L40.00013 End-monomer dynamics in semiflexible polymers, MICHAEL HINCEWSKI, XAVER SCHLAGBERGER, Physics Dept., Tech. Univ. of Munich, MICHAEL RUBINSTEIN, Dept. of Chemistry, Univ. of North Carolina, OLEG KRICHESKY, Physics Dept., Ben-Gurion Univ., ROLAND NETZ, Physics Dept., Tech. Univ. of Munich — Precise experimental observations over the last few years of end-monomer dynamics in the diffusion of double-stranded DNA have given conflicting results: one study indicated an unexpected Rouse-like scaling of the mean squared displacement (MSD) $\langle r^2(t) \rangle \sim t^{1/2}$ at intermediate times, corresponding to fluctuations at length scales larger than the persistence length but smaller than the coil size; another study claimed the more conventional Zimm scaling $\langle r^2(t) \rangle \sim t^{2/3}$ in the same time range. Spurred by this experimental controversy, we investigate the end-monomer dynamics of semiflexible polymers through Brownian hydrodynamic simulations, an improved dynamic mean-field theory, and a heuristic scaling argument [1]. Both theory and simulation point to a novel intermediate dynamical regime where the effective local exponent of the end-monomer MSD, $\alpha(t) = d \log \langle r^2(t) \rangle/d \log t$, drops below the Zimm value of 2/3 for sufficiently long chains. This deviation increases with chain length (though it does not reach the Rouse limit of 1/2), and is related to hydrodynamic effects in the slow crossover from dynamics on length scales smaller than the persistence length to dynamics on larger scales. [1] arXiv:0809.0667v1, Macromolecules in press (2008).
5:06PM L40.00014 Hydration effect on optical property of a DNA fiber: A first-principles study\textsuperscript{1}. TAKENORI YAMAMOTO, Faculty of Science, Toho University and IIS, The University of Tokyo, TSUYOSHI UDA, AdvanceSoft Corporation, TAKAHISA OHNO, National Institute for Materials Science (NIMS) and IIS, The University of Tokyo — We present a first-principles study for salvation effects on properties of a deoxyribonucleic acid (DNA) double helix fiber. The first-principles electronic structure and the molecular dynamics simulations reveal that the electronic structure of the DNA fiber is varied by the hydration amount and the deformation. The electrostatic interaction in the DNA fiber is screened by the hydration water. The screened electrostatic interaction determines the electronic structure of the DNA fiber, while the electronic structure of the water is determined by its polarized change as the result of the electrostatic response. We show that the optical conductivity is influenced by the hydration and the deformation, and that our findings agree with other theoretical results and experimental observations. In conclusion, we really stress that the solvation must be carefully taken account for simulating electronic structures and properties of DNA’s.

\textsuperscript{1}A part of this research was done in RISS project supported by RDINIT of MEXT.

5:18PM L40.00015 Supercoil Formation During DNA Melting\textsuperscript{1}. MEHMET SAYAR, BARIS AVSAROGLU, ALKAN KABAKCI OGLU, Koc University — Supercoil formation plays a key role in determining the structure-function relationship in DNA. Biological and technological processes, such as protein synthesis, polymerase chain reaction, and microarrays rely on separation of the two strands in DNA, which is coupled to the unwinding of the supercoiled structure. This problem has been studied theoretically via Peyrard-Bishop and Pollock-Scheraga type models, which include a simple representation of the DNA structural properties. In recent years, computational models, which provide a more realistic representation of DNA molecule, have been used to study the melting behavior of short DNA chains. Here, we will present a new coarse-grained model of DNA which is capable of simulating sufficiently long DNA chains for studying the supercoil formation during melting, without sacrificing the local structural properties. Our coarse-grained model successfully reproduces the local geometry of the DNA molecule, such as the 3'-5' directionality, major-minor groove structure, and the helical pitch. We will present our initial results on the dynamics of supercoiling during DNA melting.

\textsuperscript{1}Tubitak Grant No:108T553

Tuesday, March 17, 2009 2:30PM - 5:18PM — Session L41 DAMOP: Atom-Photon Interactions 413

2:30PM L41.00001 Few electron systems in a strong laser pulse. NICHOLAS VENCE, University of Tennessee, PREDRAG KRSTIC, Oak Ridge National Laboratory, ROBERT HARRISON, University of Tennessee / Oak Ridge National Laboratory — We propose a numerical procedure for investigating the dynamics of a one electron wave function in a strong, sub-femtosecond laser field. The non-perturbative time evolution method does not rely on an eigenfunction basis set but uses the multiresolution techniques for spatial discretization as described in [Harrison et. al., J. Chem. Phys. 121, 2866 (2004)]. The time propagation is done by the chin-chin time splitting method [Chin Chen, J. Chem. Phys. 114, 7338 (2001)]. The excitation and ionization cross-sections for the hydrogen atom, the oxygen ion and the hydrogen molecular ion could serve as a benchmark for future calculations and experiments due to the well controlled accuracy inherent in this numerical scheme.

2:42PM L41.00002 Theoretical study of electron momentum distribution in He tunneling ionization, LI GUO, SHENGSHENG HAN\textsuperscript{1}, JINGYUN FAN, Joint Quantum Institute, NIST and UMCP, JING CHEN, Institute of applied physics and computational mathematics — The electron scattering amplitude given by the S-matrix theory, up to the third order, can be written as

\[ S_{fi} = -i \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dt'' \left\langle \psi_{f}(p,t) \right| V_{A}(t) \left| \psi_{i}(p,t) \right\rangle - i \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' \left\langle \psi_{f}(p,t) \right| V_{G}(t,t') V_{A}(t') \left| \psi_{i}(p,t) \right\rangle, \]

with the first term describing the direct ATI process (that the initial state directly scatters to the final state), the second term describing that the electron initially scatters to the intermediate states via the laser-electron interaction (VA) and then scatters to the final state via the electron-ion interaction (V) (a rescattering ATI process), and the third term describing that the electron scatters to the final state via two cascaded ATI processes. All scattering processes are physically indistinguishable, so we assume that all divergence processes in scattering processes (corresponding to the forward scattering) can be absorbed into the first term and exclude them in the calculation, where the divergence is due to the long range Coulomb interaction (V = -1/r). We apply this method to study the He ionization and our theoretical results are qualitatively consistent with recent experimental observations.

\textsuperscript{1}Shanghai Institute of Optics and Precision Mechanics

2:54PM L41.00003 Modulation of molecular high harmonic generation by electron de Broglie wave interference. JING CHEN, Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, 100088 Beijing, China, JING YUN FAN, Joint Quantum Institute, National Institute of Standards and Technology, and University of Maryland — In the intense laser field, the amplitude for the \( n \)-th-order high harmonic generation (HHG) of a two-center molecule using the modified Lewenstein model is written as

\[ S(n) \propto \sum_{J_{n}} \langle \psi_{f}(p,t) \rangle \langle \psi_{i}(p,t) \rangle^{*} \Phi_{l}(k) \right| J_{n}(\frac{k}{\omega}) \left| \Phi_{l}(k) \right\rangle, \]

where \( m \) and \( n \) are number of photons that the electron absorbs/emits at ionization/recombination and are restricted by the energy conservation, \( n = (m \pm 1) + \frac{1}{2} \). The electron’s kinetic energy is related to photon number \( m \) and molecular ionization potential \( I_{p} \) as \( E_{k}^{2} = (m \pm 1)\omega - I_{p} \). \( E_{k} \) is parallel to \( \overrightarrow{k} \) with \( k^{2} = 2 \omega^{2} + I_{p} \) due to the bound potential acceleration effect in the recapture. \( J_{n}(k) \) is \( n \)-th order Bessel function and \( \Phi_{l}(k) \) is the amplitude of electron momentum state (Fourier transformation of the atomic wavefunction \( \phi_{l} \) in the LCAO-MO approximation).

Clearly MMHG at each order \( (n) \) is contributed by a number of momentum states, being a summation of interferences \( \langle \psi_{f}(p,t) - \psi_{i}(p,t) \rangle \) weighted by state probabilities which is affected by laser parameters. We numerically evaluate the MMHG spectra for different laser intensities and various alignment angles, the results are consistent with recent experimental observations.

3:06PM L41.00004 ABSTRACT WITHDRAWN —

3:18PM L41.00005 ABSTRACT WITHDRAWN —
3:30PM L41.00006 Entangling photons by means of the nonlinear response of quantum wells to an ultrashort pulse. MIKHAIL EREMENCHOUK, MICHAEL LEUENBERGER, University of Central Florida — Polarization-entangled photons can be produced from semiconductor bulk crystals made of CuCl through resonant hyperparametric scattering off the bound biexciton state with a yield exceeding $10^{-5}$, much higher than yields $<10^{-9}$ achieved with bulk nonlinear crystals. Here we show a different method to produce pairs of entangled photons in the short time response of a quantum well excited by a short intense pulse. At the time scales, where the biexciton effect is not yet pronounced, the Pauli exclusion principle is responsible for many-body correlations among excitons, giving rise to the production of entangled photons with a yield of around $10^{-2}$. We make use of a quantum-field theoretical two-particle density matrix to calculate the entanglement for arbitrary emission angles of the entangled pairs of photons. At the time scales, where the heavy-light hole splitting is resolved, the resonances corresponding to different two-exciton states are developing, so that a simple kinematic theory can be presented, which relates the states of the outgoing photons with the respective two-exciton states. We study remarkably strong nontrivial dependence of entanglement on the emission angles of the entangled photons and on the ellipticity parameters of the incident photons. We show that the emitted entangled 2-photon states are always in a triplet state.

1We acknowledge support from NSF ECCS-0725514 and DARPA Young Faculty Award.

3:42PM L41.00007 Two and three dimensional study of the hydrogen molecular ion $H_2^+$ confined between double boxes of spherial and spherical geometries. MARTIN MOLINAR, GERMAN CAMPOY, Departamento de Investigacion en Fisica, Universidad de Sonara — Considering first a two-dimensional system, we study the hydrogen molecular ion confined in the space between two ellipses, and then we consider its confinement in the space between two prolate spheroids. In the Born – Oppenheimer approximation, we solve numerically the Schrodinger’s equation for the above mentioned cases, using an algorithm that allows us to calculate the energies for different given values of the confinement parameters. We also consider the confinement in the region limited by two concentric circumferences and in the two-dimensional case, in the region between two concentric spherical shells. In the last two cases we use the variational method in order to estimate the energy of the ground state. Some properties of the system as the pressure exerted by the confinement, the polarizability in the approximations of Kirkwood and Buckingham and the energies of the vibrational states are calculated. The behavior of the internuclear separation is analyzed for all the geometries considered.

3:54PM L41.00008 Dipole in a Magnetic Field, Work, and Quantum Spin. ROBERT J. DEISSLER, Physics Department, Cleveland State University, Cleveland, OH — Place an atom in a nonuniform static external magnetic field and, because of the interaction between the atom’s magnetic moment and the magnetic field gradient, the atom will accelerate. An important and fundamental question, which has been neglected in the literature, is whether or not the magnetic field is doing work on the atom. It is shown that, while the magnetic field does no work on the electron-orbital contribution to the magnetic moment (the source of translational kinetic energy being the atom’s internal energy), whether or not it does work on the electron-spin contribution to the magnetic moment depends on whether the electron has an intrinsic rotational kinetic energy associated with its spin. If the electron does have a rotational kinetic energy, which is shown to be consistent with the Dirac equation, the acceleration of a silver atom in a Stern-Gerlach experiment or the emission of a photon from an electron spin-flip can be explained without requiring the magnetic field to do work. A classical dipole (a spinning charged ball) is also studied. For details please refer to R.J. Deissler, Phys. Rev. E. 77, 036609 (2008). A link to this paper, as well as other information, may be found at http://deissler.us/.

4:06PM L41.00009 Casimir force measurements between a gold sphere and a rectangular corrugated Silicon plate. YILIANG BAO, JIE ZOU, H.B. CHAN, University of Florida — The Casimir force is the interaction that results from quantum fluctuations of electromagnetic fields in vacuum and strongly depends on the shape of the boundaries that confines the electromagnetic fields. Most previous experiments involve simple geometries such as plate-sphere, two parallel plates or two cylinders, where the pair-wise summation of two-body interactions is still valid. To demonstrate the strong shape dependence of the Casimir force, we choose one of the interacting surfaces to be an array of trenches with widths ranging from 200 nm to 500 nm. Both high-aspect-ratio trenches with depth of 1 um and shallow trenches with depth of 100 nm are fabricated. The force gradient on these structures is measured with a micromechanical torsional oscillator for the separations between 150 nm and 500 nm. We observe deviations from both the pair-wise additive approximation and the proximity force approximation. The observed deviation, however, is smaller than the calculated values for perfectly conducting surfaces, possibly due to the interplay between finite conductivity and geometry effects.

4:18PM L41.00010 Distance dependence of contact potential in cylindrical-plane Casimir force measurements. QUN WEI, KEVIN MILLER, Dartmouth College, DIEGO DALVIT, Los Alamos, ROBERTO ONOFRIO, Dartmouth College — We report on the status of an experiment aimed at measuring the Casimir force in cylinder-plane geometry. In order to characterize the apparatus, we have first performed small distance electrostatic calculations. This has allowed us to better identify various general issues on the measurement of the Casimir force, such as the determination of the way the distance dependence of the contact potential $V_{0}$ is particularly crucial since its distance dependence can affect the entire data analysis procedure. We also carried on the measurements of $V_{0}$ in sphere-plane and plane-plane geometries for comparison.

4:30PM L41.00011 Optical binding force acting on two optically trapped particles. H.D. OU-YANG, MING-TZO WEI, Lehigh University — In addition to common optical manipulation setups such as an optical tweezers, the radiation forces generated by a laser can also induce chain-like arrangements of $\mu$m-sized dielectric spheres through coherent multiple scattering, through a process known as optical binding (OB). Although the forces generated through OB are on the order of piconewtons, they are still sufficient to overcome other relevant interactions in the suspension such as Van Der Waals and gravitational forces and Brownian fluctuations. The OB force oscillates from attractive to repulsive as function of interparticle separation; as observed in theoretical models and optical fields found in systems such as counter propagating lasers in dual-beam optical-fibers. Using a dual optical tweezers setup, we have measured the inter-particle OB force from two 1.5 micron diameter polystyrene particles in suspension as a function of their separation by holding them in separate optical traps. Using a calibration scheme, we have isolated the OB force from the background of hydrodynamic and Brownian forces. Using experimental measurements and theoretical predictions, we also proved that by changing the respective polarizations between parallel and perpendicular orientations of the two traps, the OB force was the only force acting on the particles.

4:42PM L41.00012 Reflection of Various Types of Waves by Layered Media. SERGIY MOCHOV, BORIS ZELDOVICH, College of Optics and Photonics / CREOL, UCF — The one-dimensional wave equation describing propagation and reflection of waves in a layered medium is transformed into the notion of an exact first-order system for the amplitudes of coupled counter-propagating waves. Any choice of such amplitudes, out of continuous multitude of them, allows one to get an accurate numerical solution of the reflection problem. We discuss relative advantages of particular choices of amplitude. We also introduce the notion of reflection strength of a plane wave by a nonabsorbing layer, which is related to the reflection intensity $R$ by $R = \tan^{2}S$. We show that the total reflection strength by a sequence of elements is bounded above by the sum of the constituent strengths, and bounded below by their difference. Reflection strength is discussed for propagating acoustic waves and quantum mechanical waves. We show that the standard Fresnel reflection may be understood in terms of the variable $S$ as a sum or difference of two contributions, one due to a discontinuity in impedance and the other due to a speed discontinuity.
4:54PM L14.00013 Gravitational Redshift and Deflection of Slow Light, JUSTIN DRESSEL, S. RAJEV, JOHN HOWELL, ANDREW JORDAN, University of Rochester — We explore the nature of the classical propagation of light through media with strong frequency-dependent dispersion in the presence of a gravitational field. In the weak field limit, gravity causes a redshift of the optical frequency, which the slow-light medium converts into a spatially-varying index of refraction. This results in the bending of a light ray in the medium. We further propose experimental techniques to amplify and detect the phenomenon using weak value measurements. Independent heuristic and rigorous derivations of this effect are given.

5:06PM L14.00014 Control of a mechanical resonator mode by cavity-enhanced light scattering, AKO CHIJOKE, JOHN LAWALL, NIST — Reaching the quantum regime of a mechanical resonator is facilitated by using a resonator with a small mass and high frequency. On the other hand, optical interferometry fails if the dimensions of the resonator are not significantly larger than the optical wavelength. Here we discuss and demonstrate an alternative optical technique employing scattering losses within an optical cavity to sense the motion of a resonator that can have dimensions well below the optical wavelength. We place a wavelength-scale mechanical resonator at the waist of a high-finesse optical cavity, lock the cavity to a resonance, and monitor the transmission. As the resonator vibrates, it modulates the cavity loss and thereby the transmitted power. We calibrate the sensitivity to resonator position by means of a known static displacement. We then sense the thermal motion of the resonator, and employ active feedback to cool, heat, and stiffen the mechanical mode.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P1 DCMP: Optoelectronic Manipulation and Control of Charges and Spins in Quantum Dots — Spirit of Pittsburgh Ballrom A

8:00AM P1.00001 Optical control of spin coherence in singly charged quantum dots, MANFRED BAYER, TU Dortmund University — The most promising candidate for implementation of quantum information technologies in semiconductors is the spin of an electron confined in a quantum dot because of its good coherence properties. Our approach is based on using an electron spin ensemble for defining a robust macroscopic quantum bit. Typically such an ensemble suffers from inhomogeneities. Using tailored pulsed laser excitation protocols this ensemble can be homogenized, such that the involved electrons appear to be identical when precessing about an external magnetic field. In this contribution problems and perspectives related to this approach will be discussed. In particular collective initialization and manipulation of the electron spin ensemble will be addressed. The use of all-optical techniques ensures that the manipulation can be performed on picosecond time scales.

8:36AM P1.00002 The quantum dot molecule from an optical point of view, DANIEL GAMMON, Naval Research Laboratory — For over ten years the techniques of single quantum dot optical spectroscopy has enabled rapid progress in the fundamental understanding of quantum dots and in the application of quantum information concepts [1]. We now apply these ever improving optical techniques to two self-assembled InAs/GaAs quantum dots that are coherently coupled through tunneling that is, a quantum dot molecule [2]. The optical spectrum of a quantum dot molecule is much richer than that of a single quantum dot. As one might expect, there is both new physics and enhanced opportunity for quantum information applications. We find that the optical spectrum of single QD molecules charged with 0, 1, or 2 electrons or holes show intriguing and unique patterns of anti-crossings and spin exchange splittings that are readily understood in terms of a few simple concepts. Closer inspection is revealing new information and opportunity, however. For example, on the fundamental side, we have recently discovered evidence that the ground state of the molecule can be an anti-bonding state when it is the hole that tunnels between the dots a new effect not found in atoms. On the quantum information side, we have engineered a quantum dot molecule in which we can simultaneously control and nondestructively measure the spin of a single electron. This solves a serious limitation in the optical control of single quantum dots. These studies are laying the groundwork necessary to enable optically controlled entanglement of two spins. Here I give an overview of our current understanding of this system from an optical point of view.

9:12AM P1.00003 Spectroscopy of Collective Modes in Few-electron Quantum Dots, SOKRATIS KALLIAKOS, Department of Materials Science and Technology, University of Crete — Quantum correlations among electrons confined in semiconductor quantum dots (QDs) are expected to lead to exotic states of matter, such as an electron molecule. In the limit of vanishing electron density, the distances between the confined electrons are rigidly fixed like those of nuclei in conventional molecules. The electronic excitations of such a molecule are quantized normal modes of roto-vibration, whose quanta have either a rigid-rotor or relative-motion character. Recent progress on the emergence of molecular roto-vibrational modes at experimentally attainable densities will be discussed. Signatures of the roto-vibrational spectrum are observed even if the localization in space of the electron wave functions is not yet fully achieved. I will present a joint experimental and theoretical investigation of the neutral electronic excitations of nanofabricated AlGaAs/GaAs QDs that contain four electrons. We use inelastic light scattering to probe electronic charge and spin excitations in an array of identical nanofabricated QDs. Spectra of low-lying excitations associated to changes of the relative-motion wave function -the analogues of the vibrational modes of a conventional molecule- do not depend on the rotational state represented by the angular momentum, which can be controlled by the application of a magnetic field. A theoretical model, based on full configuration-interaction method, offers an excellent quantitative agreement with the experimental findings. I will also demonstrate optical control of the number of electrons and lateral confining potential in our GaAs/AlGaAs QDs. This is achieved by illumination with a weak laser beam that is absorbed in the AlGaAs barrier. Precise tuning of the energy-level structure and number of electrons is manifested in the evolution of low-lying spin and charge excitations probed by inelastic light scattering. Our findings open a new venue towards the all-optical manipulation of single electrons in QDs.

9:48AM P1.00004 Quantum coherence of electron spins in semiconductor quantum dots, SANKAR DAS SARMA, University of Maryland — No abstract available.

1Work has been supported by BMBF and DFG.


3Additional affiliation: Scuola Normale Superiore, Pisa, Italy
10:24AM P1.00005 Ultrafast Coherent Control of a Single Electron Spin in a Quantum Dot

MAIKEN H. MIKKELSEN
Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — Quantum information processing schemes require fast single-qubit operations. For spin-based qubits, this involves performing arbitrary coherent rotations of the spin state on timescales much faster than the spin coherence time. While we recently demonstrated the ability to initialize and monitor the evolution of single spins in quantum dots (QDs) here we present an all-optical scheme for ultrafast manipulation of these states through arbitrary angles. The GaAs QDs are embedded in a diode structure to allow controllable charging of the QDs and positioned within a vertical optical cavity to enhance the small single spin signal. By applying off-resonant optical pulses, we coherently rotate a single electron spin in a QD up to 20 radians on picosecond timescales. We directly observe this spin manipulation using time-resolved Kerr rotation spectroscopy at T = 10K. Measurements of the spin rotation as a function of laser detuning and intensity confirm that the optical Stark effect is the operative mechanism and the results are well-described by a model including the electron-nuclear spin interaction. Using short tipping pulses, this technique enables one to perform a large number of operations within the coherence time. This ability to perform arbitrary single-qubit operations enables sequential all-optical initialization, ultrafast control and detection of a single electron spin for quantum information purposes.

Work supported by NSF and AFOSR.

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Wednesday, March 18, 2009 8:00AM - 11:00AM –
Session P2 DCMP: Critical Spin Liquids in Strongly Correlated Systems

8:00AM P2.00001 Quantum spin liquid in the spin-1/2 triangular antiferromagnet EtMe_3Sb[Pd(dmit)_2]_2, REIZO KATO, RIKEN — EtMe_3Sb[Pd(dmit)_2]_2 (Et=C_2H_5-, Me=CH_3-, dmit=C_5H_5N^-) is one of molecular conductors derived from an anion radical of the Pd(dmit)_2 molecule and closed-shell monocations (EtMe_3Sb)^(2-)(Z=N, P, As, Sb; x=0, 1, 2) [1]. A common feature of these Pd(dmit)_2 salts is a conducting anion layer where the Pd(dmit)_2 anions form a dimer unit [Pd(dmit)_2]_2^2-. Electronic structure around the conduction band can be described by a simple tight-binding calculation based on the dimer unit. At ambient pressure, all the Pd (dmit)_2 salts behave as Mott insulators where one spin is localized on each dimer. Interdimer transfer integrals indicate that the dimers form a quasi (isosceles) triangular lattice. Interdimer transfer integrals can be tuned by the choice of the cation, which deeply affects the electronic state. The EtMe_3Sb salt has a nearly regular-triangular lattice. The EtMe_3Sb cations are located between conduction layers and exhibit orientational disorder. The temperature dependence of the magnetic susceptibility is described in terms of the Padé approximant expression based on the high temperature series expansion of the antiferromagnetic spin-1/2 Heisenberg model on the triangular lattice with an exchange interaction J=220-250 K. The 13C-NMR measurements show no indication of either spin ordering/freezing or an appreciable spin gap down to 1.37 K, which is lower than 1% of J [2]. The specific heat measurements indicate gapless spin excitation. These results strongly suggest that the ground state of the EtMe_3Sb salt is a gapless spin liquid state. On the other hand, the EtMe_3Sb salt, which has also a nearly regular-triangular lattice, shows a first-order transition toward a charge separation state (2Dimer^- \rightarrow Dimer^0 + Dimer^2+) at 70 K [3].

References

8:36AM P2.00002 Spin Liquid State of in the $S = 1/2$ Hyper-kagome Antiferromagnet Na$_2$Ir$_4$O$_8$, HIDENORI TAKAGI, University of Tokyo/RIKEN — A new Ir oxide, Na$_2$Ir$_4$O$_8$, with a cation-ordered (Ir and Na) spinel structure, was discovered [1]. This compound is an S=1/2 Mott insulator with d^3 (low spin state) Ir^4+. As a result of the ordering of Ir and Na within spinel B-sites, magnetic Ir^4+ ions form a three-dimensional network of corner-sharing triangles, called hyper-kagome lattice, which provides us with a novel playground for the physics of frustration in S=1/2 hyper-kagome A new Ir oxide, Na$_2$Ir$_4$O$_8$, with a cation-ordered (Ir and Na) spinel structure, was discovered [1]. This compound is an S = 1/2 Mott insulator with d^3 (low spin state) Ir^4+. As a result of the ordering of Ir and Na within spinel B-sites, magnetic Ir^4+ ions form a three-dimensional network of corner-sharing triangles, called hyper-kagome lattice, which provides us with a novel playground for the physics of frustration in S=1/2 hyper-kagome antiferromagnet. It may be interesting to infer that hyper-kagome lattice has a chirality. The result of magnetization measurements indicates the presence of strong antiferromagnetic coupling (Curie-Weiss temperature $\theta_{CW} \sim -650$ K) between $S = 1/2$ spins. Nevertheless, we find no evidence for long range magnetic ordering in this S=1/2 hyper-kagome antiferromagnet at least down to 2 K, apparently due to the presence of geometrical frustration. The absence of long range ordering was firmly established by the persistence of 23Na NMR lines down to 2 K without intensity change [2]. These results strongly suggest that the ground state of this system is a three dimensional S = 1/2 spin liquid. Unusual spin excitations of this S = 1/2 hyper kagome system will be discussed, based on the specific heat and the NMR data at low temperatures.

References

Work done in collaboration with Y. Okamoto, S.Fujiyama, M.Nohara, H.Aruga-Katori, and K.Knoda

9:12AM P2.00003 Critical “metal”-like phases of frustrated spins and bosons in two dimensions, OLEXEI MOTRÜNICH, California Institute of Technology — I will review recent theoretical progress in understanding quantum phases of 2D correlated boson or spin systems which exhibit “Bose-metal” type phases with gapless excitations residing on surfaces in momentum space. A spin liquid phase with a Fermi surface of spinons is one example of interest, being potentially relevant to the organic spin liquid materials $\kappa$-(ET)$_2$Cu$_2$(CN)$_3$ and EtMe_3Sb[Pd(dmit)_2]_2. I will discuss frustrated spin and boson models with ring exchanges that may stabilize such phases, in particular in the vicinity of the Mott transition as is the case in the organic materials.

9:48AM P2.00004 Gapless spin liquids on the three dimensional hyper-kagome lattice of Na$_2$Ir$_4$O$_8$, YONG BAEK KIM, University of Toronto — Recent experiments indicate that Na$_2$Ir$_4$O$_8$, a material in which s=1/2 iridium local moments form a three dimensional network of corner-sharing triangles, may have a quantum spin liquid ground state with gapless spinon excitations. Using a combination of various theoretical approaches, we propose a quantum spin liquid with spinon Fermi surfaces as a favorable candidate for the ground state of the Heisenberg model on the hyper-kagome lattice of Na$_2$Ir$_4$O$_8$. We also present a theory of the bandwidth-controlled metal-insulator transition that may occur as a pressure-tuned transition in this material. We discuss our predictions in relation to the current and future experiments.
10:24AM P2.00005 Numerical Evidence of Gapless Spin Liquids on Ladders\textsuperscript{1}, DONNA SHENG, California State Univ. Northridge — I will present numerical evidence of strong-coupling phases for quasi-one-dimensional systems as ladder descendants of candidate models for 2D Bose metal and spin liquid states which possess surfaces of gapless excitations. I will discuss the phase diagrams for two concrete models (square lattice boson and triangular lattice spin models with ring-exchange) based on controlled numerical approaches (DMRG and ED), where such strong-coupling phases are realized in a wide regime of parameters. A close comparison between numerical results and slave-particle descriptions will allow us to characterize these phases in detail and identify signatures reflecting the parent 2D states.

\textsuperscript{1}Supported by NSF and DOE.

Wednesday, March 18, 2009 8:00AM - 10:24AM — Session P3 DCMP: Fe-based Superconductors: Correlation Effects 301/302

8:00AM P3.00001 ARPES studies of the electronic structure of Fe-based superconductors\textsuperscript{1}, DONGHUI LU, Stanford University — The recent discovery of superconductivity in Fe-based layered compounds has created renewed interest in high temperature superconductivity. With a superconducting transition temperature as high as 55 K, this discovery provides a new direction to understand the essential ingredients for achieving a high superconducting transition temperature. In this talk, I will present our recent angle-resolved photoemission spectroscopy (ARPES) studies on LaOFeP and (Ba,K)Fe\textsubscript{2}As\textsubscript{2} systems, with special emphasis on the basic electronic structure of the parent compounds. For LaOFeP, quantitative agreement can be found between our ARPES data and the LDA band structure calculations, suggesting that a weak coupling approach based on an itinerant ground state may be more appropriate for understanding this new superconducting compound [1]. On the other hand, the picture for (Ba,K)Fe\textsubscript{2}As\textsubscript{2} can be found between our ARPES data and the LDA band structure calculations, suggesting that a weak coupling approach based on an itinerant ground state may be more appropriate for understanding this new superconducting compound [1].

1The work is supported by DOE Office of Basic Energy Science.

8:36AM P3.00002 Charge dynamics in the normal state of the iron oxypnictide superconductor LaFePO\textsubscript{1}, M. M. QAZILBASH, University of California - San Diego — Many-body interactions in materials govern diverse and complex phenomena like high-T\textsubscript{c} superconductivity, density wave instabilities and metal-insulator transitions. Infrared spectroscopy is an ideal tool for identifying the fingerprints of the various interactions in a material. We present infrared and optical properties in the normal state of in-plane oriented single crystals of the iron oxypnictide superconductor LaFePO. Prominent Drude peaks and low scattering rates indicate the presence of coherent quasiparticles. We find that this metal has a relatively low carrier density compared to MgB\textsubscript{2}, for example. An important result is that the Drude spectral weight i.e. the kinetic energy of itinerant quasiparticles is reduced by correlation effects to 50% of the band theory value. Even though LaFePO is among the most conducting of the iron-pnictides, we find that electronic correlations cannot be ignored in any realistic physical description of this material. We classify LaFePO as a moderately correlated metal.

1This work was performed in collaboration with J. J. Hamlin, R.E. Baumbach, M. B. Maple, Lijun Zhang, D. J. Singh, and D. N. Basov. Support from the National Science Foundation via grant NSF-DMR0705171 is gratefully acknowledged.

9:12AM P3.00003 Electronic Correlations and Magnetic Frustration in the Iron Pnictides\textsuperscript{1}, QIMIAO SI, Rice University — An important question about the high T\textsubscript{c} iron pnictides is the extent to which they are strongly correlated. Based on the fact that they are “bad metals,” we propose that these materials are in proximity to a Mott insulator [1,2]. In other words, the degree of the electronic correlations here is closer to that of intermediate-coupled metallic systems like V2O3, which lies near the Mott transition, rather than that of simple antiferromagnetic metals such as Cr. Consequently, we model the incoherent electronic excitations in terms of localized moments, whose superexchange interaction contain the competing nearest-neighbor (J1) and next-nearest-neighbor (J2) components [1]. The magnetic frustration of the J1-J2 model in the relevant parameter range leads to a (pi,0) antiferromagnet and a reduced ordered moment. The model also features an Ising transition that naturally yields a structural phase transition. All these results are consistent with the neutron scattering results. With the coupling of the local moments to the coherent electronic excitations, the strength of the antiferromagnetic order is tuned, leading to a magnetic quantum critical point [2]. The ordered moment should therefore vary across the undoped iron arsenides. In addition, the magnetic quantum criticality can be probed by P doping for As in the parent iron pnictides, where the disruption to the quantum criticality caused by superconductivity is likely to be less compared to the electron or hole doped cases. Finally, the implications of the electronic correlations and magnetic frustration on the multi-band superconductivity will be briefly discussed.

\textsuperscript{1}In collaboration with E. Abrahams, J. Dai, P. Goswami, P. Nikolic and J.-X. Zhu. Supported by NSF and the Welch Foundation.

9:48AM P3.00004 Pairing symmetry and Antiferromagnetic Exchange Coupling in Fe-Based Superconductors\textsuperscript{1}, JIANGPING HU, Purdue University — I discuss the existence of strikingly identical paradigms applicable to both cuprates and iron-based superconductors in understanding magnetism, superconductivity and the interplay between the two. The magnetic states and transitions in iron-based superconductors are well described by a J\textsubscript{1} \(-\) J\textsubscript{2} \(-\) J\textsubscript{3} magnetic exchange model where J\textsubscript{1}, J\textsubscript{2} and J\textsubscript{3} are nearest neighbour, next nearest neighbour and inter-layer couplings respectively. Differing from the t-J model for cuprates where d-wave pairing symmetry is favored, the magnetic exchange in the iron based superconductors predicts an unconventional s-wave \(\cos k_x \cos k_y\) pairing. I will show that the predicted pairing symmetry is supported by many experimental results, and also discuss new predictions associated with the pairing symmetry.

References:

\textsuperscript{1}The work is supported by NSF under grant No. PHY-0603759.
reverse osmosis and nanofiltration membranes used for water purification are real-world examples of nanoscale functional materials: the active layer is only ~100 nm thick. Because the active layer is formed by a process of interfacial polymerization, the structure and composition of the membrane is highly inhomogeneous and even such basic physical and chemical properties as the atomic density, swelling in water, the distribution of charged species between water and membrane, and the mobility of water and ions, are poorly understood. We are using Rutherford backscattering spectrometry (RBS) to determine the composition, roughness, and thickness of the membrane; reveal the surprisingly high solubility of salt ions in the polymer active layer; analyze the acid-base chemistry of charged functional groups; and determine the degree of polymer cross-linking. Measurements of mass-uptake and adsorption-induced mechanical stress of membranes in humid air enable us to determine the water solubility, specific volume of water, and the mechanical strength of the membrane. Comparisons between these equilibrium data and the permeability of the membrane to water and salts show that the mobility of water molecules in the membrane approaches the mobility of bulk water, and that the rejection of salt ions is accomplished by low mobility, not low solubility. My collaborators in this work are Xijing Zhang, Orlando Coronell, and Prof. Benito Mariñas.

1 supported by the NSF through The Center of Advanced Materials for the Purification of Water with Systems

8:36AM P4.00002 High Flux Nanofibrous Membranes for Water Purification1, BENJAMIN HSIAO, Stony Brook University — Recently, nanofibrous materials have been made more readily available in large part due to advances in electro-spinning and related technologies, including the use of a combination of electrostatic and gas-blowing forces. The non-woven structure has unique features, including interconnected pores, very large surface-to-volume ratio, and ease of surface modifications which enable such scaffolds to have many biomedical and industrial applications. The chemical composition of electrosprun membranes can be adjusted by using different polymers, polymer blends or nanocomposites, made of organic or inorganic materials. In this talk, we demonstrate a breakthrough technology on the fabrication of high-flux water purification by carbon nanofibrous membranes. The breakthrough incorporates two new and unique concepts of the membrane design: (1) the replacement of the conventional flux-limited porous substrate with a highly porous nanofibrous scaffold, and (2) the creation of a very thin, strong and functional nanocomposite barrier layer, imbedded with interconnected and directed water channels. Preliminary experiments on the hierarchical design and assembly of this unique nanofibrous membrane have already revealed very promising potentials. By using a hydrophilic nanocomposite barrier layer, an asymmetric electrosprun nanofibrous mid-layer scaffold and a non-woven microfibrinous support, the flux rate of this not-yet-optimized membrane system is 3-10 times better than that of the best among all known conventional ultrafiltration/nanofiltration media without losing the high rejection and low fouling criteria.

1This is a joint collaboration with Ben Chu. The work is supported by ONR.


9:48AM P4.00004 Carbon Nanotube Membranes for Water Purification1, OLIGICA BAKAJIN, Biosciences and Biotechnology Division, PLS, Lawrence Livermore National Laboratory — Carbon nanotubes are an excellent platform for the fundamental studies of transport through channels commensurate with molecular size. Water transport through carbon nanotubes is also believed to be similar to transport in biological channels such as aquaporins. I will discuss the transport of gas, water and ions through microfabricated membranes with sub-2 nanometer aligned carbon nanotubes as ideal atomically-smooth pores. The measured gas flow through carbon nanotubes exceeded predictions of the Knudsen diffusion model by more than an order of magnitude. The measured water flow exceeded values calculated from continuum hydrodynamics models by more than three orders of magnitude and is comparable to flow rates extrapolated from molecular dynamics simulations and measured for aquaporins. More recent reverse osmosis experiments reveal ion rejection by our membranes. Based on our experimental findings, the current understanding of the fundamentals of water and gas transport and of ion rejection will be discussed. The potential application space that exploits these unique nanofluidic phenomena will be explored. The extremely high permeabilities of these membranes, combined with their small pore size will enable energy efficient filtration and eventually decrease the cost of water purification.

In collaboration with Francesco Fornasier, Biosciences and Biotechnology Division, PLS, LLNL, Livermore, CA 94550; Sangil Kim, NSF Center for Biophotonics Science & Technology, University of California at Davis, Sacramento CA 95817; Jung Bin In, Mechanical Engineering Department, UC Berkeley, Berkeley CA 94720; Hyung Gyu Park, Jason K Holt, and Michael Stadermann, Biosciences and Biotechnology Division, PLS, LLNL; Costas P. Grigoropoulos, Mechanical Engineering Department, UC Berkeley; Aleksand Noy, Biosciences and Biotechnology Division, PLS, LLNL and School of Natural Sciences, University of California at Merced.

1Prepared by LLNL under Contract DE-AC52-07NA27344, with funding from LLNL’s LDRD program, DARPA, & NSF.

10:24AM P4.00005 Hierarchical Fiber Structures Made by Electrospinning Polymers, DARRELL H. RENEKER, The University of Akron — A filter for water purification that is very thin, with small interstices and high surface area per unit mass, can be made with nanofibers. The mechanical strength of a very thin sheet of nanofibers is not great enough to withstand the pressure drop of the fluid flowing through. If the sheet of nanofibers is made thicker, the strength will increase, but the flow will be reduced to an impractical level. An optimized filter can be made with nanometer scale structures supported on micron scale structures, which are in turn supported on millimeter scale structures. This leads to a durable hierarchical structure to optimize the filtration efficiency with a minimum amount of material. Buckling coils and pendulum coils spanning dimensions from a few microns to a few centimeters can be collected from a single jet by controlling the position and motion of a collector. Attractive routes to the design and construction of hierarchical structures for filtration are based on nanofibers supported on small coils that are in turn supported on larger coils, which are supported on even larger overlapping coils. "Such top-down" hierarchical structures are easy to make by electrospinning. In one example, a thin hierarchical structure was made, with a high surface area and small interstices, having an open area of over 50%, with the thinnest fibers supported at least by 10 microns.

1Tao Han, Darrell R Reneker, Alexander L. Yarin, Polymer, Volume 48, issue 20 (September 21, 2007), p. 6064-6076.
8:00AM P5.00001 Inertial Particles in Turbulent Flows and the Clustering Instability of Interstellar Dust, PAOLO PADOAN, University of California, San Diego — The dynamics of dust grains in turbulent flows plays an important role in many astrophysical processes. I will review the problem of the formation of planetesimals (precursors of full-fledged planets) in turbulent circumstellar disks. I will then discuss some fundamental aspects of the physics of heavy particles in turbulent flows, and specifically the phenomenon of small scale clustering, an effect verified by laboratory experiments and in situ terrestrial cloud sampling. I will present results of large numerical simulations of particle-laden compressible turbulence, including statistics of clustering and of particle velocity differences.

8:36AM P5.00002 Multiscale modeling of the human arterial tree on the TeraGrid, GEORGE KARNAĐAKIS, Brown University — A multiscale model of the human arterial tree will be presented consisting of the macrovascular network (MaN, arteries above 1-2 mm), the mesovascular network (MeN, arterioles above 10 micro-m) and the microvascular network (MiN, capillaries). Coupling conditions between the MaN-MeN-MiN will be discussed and three different methods in modeling each network will be presented. Specific examples will be shown for the intracranial arterial tree for healthy subjects but also for patients with hydrocephalus.

9:12AM P5.00003 Terascale Direct Numerical Simulations of Turbulent Combustion, JACQUELINE CHEN, Sandia National Laboratories — The rapid growth in computational power in the past decade has presented both opportunities and challenges for high-fidelity simulations of turbulent reacting flows. The advent of terascale computing power has made it possible to glean fundamental physical insight into fine-grained “turbulence-chemistry” interactions in simple laboratory-scale turbulent flames from direct numerical simulation at moderate Reynolds numbers with detailed chemistry. Recent DNS results are presented to elucidate the role of autoignition and large-eddy mixing on the stabilization of a lifted ethylene-air jet flame in a heated coflow. The role of scalar dissipation rate on modulating ignition delays or lift-off heights is discussed. The simulations were performed at a jet Reynolds number of 10,000 and required 1.3 billion grid points to resolve the turbulence and flame structure. In a second related topic, the morphology of the scalar dissipation rate field in a turbulent jet flame is examined using topological methods, in particular the Morse-Smale Complex, which provides a natural segmentation of dissipation rate elements or “features.” These features are tracked in time, and conditional feature statistics are presented.

9:48AM P5.00004 Prediction and predictability of hurricanes with high-performance computers and cloud-resolving ensembles, FUQING ZHANG, Penn State University — This talk will be primarily devoted to the use of high-performance computing facilities to perform ensemble-based state estimation of hurricanes with cloud-resolving numerical weather prediction models. I will be sharing our recent experience in using approximately 30,000 cluster cores simultaneously at the Texas Advanced Computing Center which successfully assimilates high-resolution airborne Doppler radar observations in realtime and subsequently delivers 2 deterministic and 60-member ensemble forecasts running at 4.5/1.5-km effective horizontal grid spacings in a timely fashion. Since the predictability of hurricanes may be fundamentally limited by chaotic moist convection and subsequent upscale error growth, I would advocate that besides the need of continuously improving the hurricane forecast models and ingesting high-resolution observations into the models to better initialize the storm, the hurricane state estimation is fundamentally probabilistic that demands cloud-solving ensemble-based data assimilation and forecasting. Improvements of forecast models may come from ever increasing computer power to better resolve the storms numerically and from improved fundamental understanding of the dynamics and impact of subgrid-scale turbulence in hurricanes. Improvements of better state estimation may also come from development of new theories that are applicable for high-dimensional, non-linear, non-Gaussian dynamic systems such as in hurricanes.

1Supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences and the Office of Advanced Scientific Computing Research of the Department of Energy.

10:24AM P5.00005 On the two-way interactions between dispersed particles and turbulent flows, SAID ELGHOBASHI, Mechan. and Aerospace Engineering Department, University of California, Irvine — Particle-laden turbulent flows are ubiquitous in nature (e.g., dust storms on Earth and Mars) and in industrial applications (e.g., liquid fuel and pulverized coal sprays in combustion chambers). Experimental and numerical studies of these flows are quite challenging due to the wide spectra of length- and time-scales of the dispersed particles in addition to the spectra of scales intrinsic to the carrier fluid turbulence. The two-way nonlinear interactions between the dispersed particles and the turbulence result in complex multi-scale physical phenomena. The lecture focuses on the physical mechanisms of the two-way interactions between dispersed spherical particles and simple turbulent flows using Direct Numerical Simulation (DNS). Particles whose diameter is smaller than the Kolmogorov length scale of turbulence are simulated as point particles. Results of particle-laden isotropic and homogeneous shear turbulent flows are presented. Particles with diameter larger than the Kolmogorov length scale are fully resolved using the Immersed Boundary method. Results of fully resolved particle-laden isotropic turbulence are presented.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P6 DAMOP: Ultracold Gases with Dipolar Interactions

8:00AM P6.00001 Ultracold polar molecules, SILKE OSPELKAUS, JILA, NIST and University of Colorado — Polar molecules — molecules exhibiting a permanent electric dipole moment — have bright perspectives as systems with long-range and anisotropic interaction. These interactions have been the basis for numerous exciting theoretical proposals ranging from ultra-cold chemistry, precision measurements, quantum phase transitions to novel systems for quantum information processing and quantum control with external magnetic and electric fields. We will present our recent work on the creation and manipulation of polar molecules exhibiting a permanent electric dipole moment, which we measure with Stark spectroscopy to be 0.566(17) Debye.


8:36AM P6.00002 Effects of magnetic dipolar interactions on collective modes and instabilities of alkali BECs, EUGENE DEMLER, Harvard University — In this talk I will review the phenomenon of roton softening in systems with dipolar interactions. Special emphasis will be on magnetic dipolar interactions in Bose condensates of alkali atoms, when fast Larmor precession and spin dynamics strongly modify the character of unstable modes. I will also discuss the enhancement of roton softening in multilayer stacks of two dimensional condensates. Implications of these theoretical results for recent experiments with Rb-87 and K-39 atoms will be discussed.
Dynamics and coherence in a collapsing dipolar BEC

Axel Griesmaier, University of Stuttgart — Chromium atoms in a Bose-Einstein condensate (BEC) interact – in addition to s-wave scattering – via magnetic dipole-dipole interaction. Although the magnetic forces between the atoms which carry a large magnetic moment of 6 Bohr magnetons are still rather weak, they can become the dominant interaction when a Feshbach resonance is used to reduce the contact interaction to zero [1]. In this regime, the stability of a chromium Bose-Einstein condensate depends on the geometry of the trap. This is an intrinsic and unique effect of an anisotropic interaction. We have measured the stability diagram of such a dipolar BEC by exploring the border between stable and unstable regions [2]. When we cross this border with an initially stable condensate by a sudden change of the scattering length into the unstable regime, we observe the collapse and subsequent explosion due to dipole-dipole interaction [3].

The anisotropy of the underlying interaction reveals in the formation of a non-trivial structure during the collapse. I will discuss the dynamics of the collapse depending on variable distance. The coexistence of translational symmetry breaking, characteristic of a solid, and long-range phase coherence, characteristic of a superfluid, are hallmarks of the sought-after supersolid phase.

1Work performed jointly with J. Guzman, S. Leslie, K. Murch, F. Serwane, and M. Vengalattore, and supported by DARPA/ARO, LBNL and NSF.

Condensed Matter Physics and Quantum Simulations with Cold Polar Molecules and Rydberg Atoms

Peter Zoller, University of Innsbruck — Polar molecules prepared in their electronic and vibrational ground state are characterized by large dipole moments associated with rotational excitations. This gives rise to large dipole-dipole interactions between molecules, which can be manipulated with external DC and AC microwave fields. The possibility to tune these strong, long-range and anisotropic interactions, combined with the trapping in reduced dimensions, raises interesting prospects for cold ensembles of polar molecules as strongly correlated condensed matter system, i.e. provides analog quantum simulation of strongly interacting systems and quantum phases. Specific examples to be discussed include the engineering of various spin and Hubbard models for polar molecules in optical lattices, e.g. the Kitaev model and three body interactions, and the tailoring effective molecular interaction potentials based on “blue-shields” with microwave fields. Furthermore, dipolar gases in 1D and 2D trapping geometries can form self-assembled lattice structures in single layer and bilayer systems. In addition, a mixture of cold atoms and polar molecules forming a self-assembled lattice gives rise to a new realization of Hubbard models with widely tunable lattice parameters and small lattice spacing, which represents a systems with both strong correlation and phonon dynamics. Extremely strong dipolar or Van der Waals interactions can also be obtained in cold atomic gases excited to Rydberg states. We will briefly discuss new ideas of developing a digital quantum simulator for spin models. It is based on performing a stroboscopic sequence of many particle quantum gates based on manipulating dipolar interactions between groups of Rydberg atoms in large spacing optical lattices.

Wednesday, March 18, 2009 8:00AM - 10:24AM –
Session P7 FEd FPS: Forging Effective Partnerships with Your Local Science Center: Outcomes from the Workshop on University/Science Center Collaborations

Lessons Learned from the APS/TFI Workshop on University/Science Center Collaborations: Outreach Targets for Potential Partners from Other Local Science Centers

David Statman, Allegheny College — On May 31 – June 1, 2008, The Franklin Institute (TFI) hosted the American Physical Society/Franklin Institute Workshop on University/Science Center Collaborations. This Workshop brought together forty leaders from science centers, universities, and federal funding agencies to explore what works and what doesn’t work in university-science center collaborations. The goal was to explore the outreach motivations of academic institutions, their scientists and students, the characteristics and needs of small vs. large science centers, and the goals for and outcomes expected from reaching out to the general public from the perspectives of universities and science centers. The result was a convergence of viewpoints on how a good collaboration is established, built upon, sustained, and evaluated.

University Perspectives on Science Center/University Interactions

Leo Kadonoff, University of Chicago — A program bringing graduate students into science museums is described. Practical, nuts and bolts, methods for making the program work are outlined. Questions are asked about the somewhat uncomfortable relation between graduate education, research, and informal education.
9:12 AM P7.00003 University/Science Center Collaborations (A Science Center Perspective): Developing an Infrastructure of Partnerships with Science Centers to Support the Engagement of Scientists and Engineers in Education and Outreach for Broad Impact, ERIC MARSHALL, Vice President, Strategic Partnerships and Innovation, Director, TryScience.org and VoITS (Volunteers TryScience) — Science centers, professional associations, corporations and university research centers share the same mission of education and outreach, yet come from “different worlds.” This gap may be bridged by working together to leverage unique strengths in partnership. Front-end evaluation results for the development of new resources to support these (mostly volunteer-based) partnerships elucidate the factors which lead to a successful relationship. Maintaining a science museum-scientific community partnership requires that all partners devote adequate resources (time, money, etc.). In general, scientists/engineers and science museum professionals often approach relationships with different assumptions and expectations. The culture of science centers is distinctly different from the culture of science. Scientists/engineers prefer to select how they will ultimately share their expertise from an array of choices. Successful partnerships stem from clearly defined roles and responsibilities. Scientists/engineers are somewhat resistant to the idea of traditional, formal training. Instead of developing new expertise, many prefer to offer their existing strengths and expertise. Maintaining a healthy relationship requires the routine recognition of the contributions of scientists/engineers. As professional societies, university research centers and corporations increasingly engage in education and outreach, a need for a supportive infrastructure becomes evident. Work of TryScience.org/VoITS (Volunteers TryScience), the MRS NISE Net (Nanoscale Informal Science Education Network) subcommittee, NRCEN (NSF Research Center Education Network), the IBM On Demand Community, and IEEE Educational Activities exemplify some of the pieces of this evolving infrastructure.

9:48 AM P7.00004 Perspective of NSF-MPS Program Directors on Educational Outreach, DANIELE FINOTELLO, National Science Foundation — The National Science Foundation Broader Impacts review criterion (often known as Criterion 2) has been subject to much discussion since first implemented by NSF. The broader impact of different proposals can vary widely, based on different factors such as the particular research activities proposed, the interests of the PI(s), the type of institution involved in the proposal, and the different opportunities available on the local area, to name just a few. In this talk the Broader Impacts review criterion will be discussed from the viewpoint of the NSF Program Officers and will include different examples of potential Broader Impact activities. In Collaboration with Uma Venkateswaran, and Kathleen V. McCcloud.

Wednesday, March 18, 2009 8:00 AM - 11:00 AM –

Session P8 FHP: Centenary of Lev Landau 414/415

8:00 AM P8.00001 Lev Landau: A View from the West, PIERRE HOHENBERG, New York University — The tragic accident which ended Landau’s scientific career at an early age meant that Lev Landau was known personally to only a small number of western scientists. His remarkable influence on twentieth century physics thus came from his published work and indirectly from the members of the famed Landau school, who are so well represented at this Symposium. Regarding the published work, I would distinguish three distinct ways in which Landau’s influence has been felt. The most obvious is the set of seminal papers on a broad set of topics ranging from Landau diamagnetism, to the phonon-roton theory and two-fluid hydrodynamics of He, Fermi-liquid theory and zero sound, the theory of second-order phase transitions, the Landau-Hopf theory of fluid turbulence and many more. The second class of contributions consists of the famed Landau-Lifshitz Course of Theoretical Physics, which first appeared in the West in the late fifties and early sixties. In many ways the third aspect of Landau’s influence, although more difficult to define, is probably even more significant. This is Landau’s pervasive presence in a large number of the major theoretical advances in condensed matter and statistical physics throughout the second half of the twentieth century. So many major developments can be viewed as elaborations, advances and - yes - corrections to the foundational theories and points of view laid down by Landau. One example is the theory of superfluidity in Bose liquids, for which one may ask why Landau resisted London’s explanation in terms of Bose condensation, which has turned out to be important after all. A second example is the Fermi liquid theory and important later developments stemming from superfluid transitions or effects of strong correlations. A third example is the theory of second-order phase transitions which lays the foundations for the study of critical phenomena using the renormalization group. In each case one marvels at the important foundational role played by Landau’s work and one may ask to what extent he anticipated the later developments. It is hoped that the subsequent speakers might address some of these questions.

8:36 AM P8.00002 Landau and theory of quantum liquids, LEV PITAEVSKII, CNR INFN-HEC, University of Trento, Trento, Italy and Kapitza Institute for Physical Problems, Moscow, Russia — General conceptions and history of the Landau Theory of superfluidity and the Theory of Fermi liquid will be discussed.

9:12 AM P8.00003 Landau and Theory of Phase Transitions, VALERY POKROVSKY, Texas A&M University — Landau’s theory of phase transitions is probably his most general and most influential work. I describe history of its creation, its basic ideas and their developments and extensions and its deep influence on modern science.

The DOE support through the grant DE-FG02-06ER46278 is acknowledged.

9:48 AM P8.00004 Landau and Feynman diagrams, IGOR DZYALOSHINSKII, University of California, Irvine — Landau considered the Feynman diagrams and the Dyson concept of their visual summation as a breakthrough in the physics of particles. This visual perception in his opinion activated the person intuition. In this intuitive way Landau introduced the concept of partial summation which led to major results in the particle physics and the condensed matter theory. Some of his and of the members of his school results will be presented in a pure visual way.

10:24 AM P8.00005 Landau’s Contributions to Applied Physics, ROAUL SAGDEEV, University of Maryland — No abstract available.

Wednesday, March 18, 2009 8:00 AM - 10:48 AM –

Session P9 GSNP: Jamming: Theory and Experiment I 303

8:00 AM P9.00001 Cooperative Particle Dynamics in the Manhattan Model, PRASANTA PAL, Department of Applied Physics, Yale University, COREY O’HERN, JERZY BLAWZDZIEWICZ, Department of Mechanical Engineering, Yale University, O’HERN GROUP TEAM, BLAWZDZIEWICZ GROUP TEAM — We study Brownian dynamics of hard rods in a Manhattan-like traffic grid, in which a series of narrow one-dimensional horizontal and vertical channels intersect at right angles, and particles are forbidden from turning at the intersections. We measure the intermediate scattering function (ISF) and mean-square displacement (msd) as a function of packing fraction φ and determine φg at which dynamical arrest occurs as a function of the system size, number of intersections, and topology of the grid. As a particular example, we explicitly characterize the cooperative particle dynamics required for structural relaxation for symmetric systems in which all lobes between junctions contain the same number of particles. In these systems, we predict the scaling behavior of the structural relaxation time and self-diffusion coefficient versus φg — φ. We will also quantify the extent to which these systems age and determine whether there is a characteristic number of junctions above which glassy dynamics occurs.
8:12AM P9.00002 Universal Scaling Relation Near Point J. THOMAS HAXTON, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania — Recently, several studies (P. Olsson and S. Teitel. Phys. Rev. Lett. 99, 178001 (2007); T. Hatano, arXiv:0803.2296; L. Berthier and T. A. Witten. arXiv:0810.4405) have indicated the existence of a dynamical phase transition at or near Point J, the point at zero temperature, zero shear stress, and a critical density where repulsive amorphous sphere packings lose rigidity. However, a universal scaling relation connecting the rheology of the jammed solid to that of the viscous liquid has been lacking. We control the temperature, strain rate, and pressure in molecular dynamics simulations to show that the steady-state rheology is described by a universal scaling relation near Point J.

1Supported by NSF-DMR-0605044.

8:24AM P9.00003 Scaling of Rheology Near the Colloidal Jamming Transition. ZEXIN ZHANG, ANINDITA BASU, THOMAS HAXTON, ANDREA LIU, ARJUN YODH, University of Pennsylvania — Recent simulations have proposed that the zero-temperature, zero-shear-stress jamming transition can be understood in the framework of critical phenomena, and thus can be described by various asymptotic scaling laws. We carry out rheology experiments in the vicinity of the jamming transition to study the scaling of flow properties of a bidisperse colloidal soft sphere system. We find, both below and above the jamming transition, a scaling collapse of the rheological data when the shear stress and shear rate are rescaled by proximity to the jamming transition. We extract critical scaling exponents and compared with simulations. C. S. O’Hern et al. Phys. Rev. E 68, 011306 (2003). P. Olsson, S. Teitel, Phys. Rev. Lett., 99, 178001 (2007). T. Hatano, arXiv:0803.2296v4 (2008), arXiv:0804.0477v2 (2008)

8:36AM P9.00004 Quenched Disorder as a Fourth Axis to the Jamming Phase Diagram. CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory, EVAN GROOPMAN, ZOHAR NUSSINOV, Washington University - St. Louis, CHARLES REICHHARDT, Los Alamos National Laboratory — We propose that the general jamming phase diagram proposed by Liu and Nagel [Nature 396, 21, 1998] as a function of shear, density and temperature could also have a fourth axis which is the density of quenched disorder. This could represent jamming in porous media. Using numerical simulations we show that the density at which jamming occurs in a two-dimensional system of disordered disks decreases as the amount of quenched disorder in the sample increases. We argue that when the jamming correlation length is on the same length scale as the average distance between disorder sites, the system will jam.

8:48AM P9.00005 Critical behavior from geometric confinement in shear thickening suspensions. ERIC BROWN, University of Chicago, HEINRICH JAEGER, University of Chicago — We performed rheometry measurements on shear thickening suspensions. The viscosity is measured as a shear stress over shear rate in the shear thickening region to have divergent scalings of both the magnitude and slope at a critical packing fraction $\phi_c$. The yield stress also has a divergent scaling at $\phi_c$. This is qualitatively different from jamming models in which the yield stress grows gradually from an onset packing fraction. The value of $\phi_c$ depends only on particle shape and equals 0.56 for hard spheres, corresponding to random loose packing and the onset of dilation.

9:00AM P9.00006 Stress Fluctuations and Nonlinear Dynamical Modes Near Jamming. DAVID A. EGOLF, Department of Physics; Georgetown University, EDWARD J. BANIGAN, Dept of Physics and Astronomy; Univ of Pennsylvania — The jamming transition is often considered a dynamical transition, but how to properly and quantitatively characterize the changes in dynamical behavior is an open question. We perform numerical simulations of a two-dimensional sheared granular layer over a range of packing fractions spanning the transition. Within these simulations, we calculate a partial spectrum of Lyapunov exponents and vectors, which (at least in one sense) is an optimal decomposition of the dynamics of the system. We find that the Lyapunov exponents and vectors corresponding to the most important dynamical modes of the system tend to localize in space and time near important physical events, such as cooperative rearrangements or redistributions of stresses. In addition, we find that the magnitudes of Lyapunov exponents are directly linked to the size of relative stress fluctuations of the system. At high densities, the system changes from chaotic to non-chaotic, and we measure dynamical time and length scales that diverge as the system jams.

9:12AM P9.00007 From Spheres to Ellipsoids: The Story of the Density of States1. ZORANA ZERAVCIC, Institute Lorentz, University of Leiden and The James Frank Institute, University of Chicago, NING XU, Department of Physics and Astronomy, University of Pennsylvania and The James Frank Institute, University of Chicago, SIDNEY R. NAGEL, The James Frank Institute, University of Chicago, ANDREA J. LIU, Department of Physics and Astronomy, University of Pennsylvania — Packings of frictionless ellipsoids have not only captured the imagination of the public, but also bring up a number of fundamental issues regarding the properties of jammed media. For instance, the average contact number $Z$ is turned on. Here we study the vibrational spectra of soft ellipsoids both as a function of density and $\epsilon$. Our spectra show a two-band structure. For small aspect ratios there is first a rotational band, then a gap and then a second band of translational character. As we increase the aspect ratio, the gap closes and there is first a rotational band, then a gap and then a second band of translational character. In addition, we find that the magnitudes of Lyapunov exponents depend only on particle shape and equals 0.56 for hard spheres, corresponding to random loose packing and the onset of dilation.

1We acknowledge support from Chicago MRSEC and Dutch physics foundation FOM.

9:24AM P9.00008 Growing length scale in gravity-driven dense granular flows. SHUBHA TEWARI, University of Massachusetts, Amherst, MELANIE FINN, Mount Holyoke College, ALLISON FERGUSON, University of Toronto, BULBUL CHAKRAVARTY, Brandeis University — We report on simulations of a two-dimensional, dense, bidisperse system of inelastic hard disks falling down a vertical tube under the influence of gravity. We examine the approach to jamming as the average flow of particles down the tube is slowed by making the outlet narrower. Defining coarse- grained velocity and stress fields, we find a length scale and a time scale can be extracted from two-point spatial and temporal correlations of these fields. Both length and time scales are found to grow as jamming is approached in an ongoing effort to understand the origin of the growing length and time scales, we have been investigating velocity profiles and distributions, and we will report on these results.

1 S. Tewari, B. Tithi, A. Ferguson and B. Chakrabortty, arXiv:0806.2413
9:36AM P9.00009 Experimental Study of the 2D Jamming Transition, XIANG CHENG, The University of Chicago — We can study a jammed system of particles by following a loosely-packed configuration as the individual particles increase their size until all the particles are constrained by their neighbors. Because tapioca pearls swell to over twice their initial diameter when submerged in water, they offer an ideal medium with which to study properties of the jamming transition in the presence of frictional interactions. Using an array of ~10,000 tapioca pearls, we study several static and dynamic signatures of the two-dimensional jamming transition. The amplitude of the first peak of the pair-correlation function changes non-monotonically as the packing fraction of the system increases. This is consistent with recent experiments in a colloidal system of NIPA particles at finite temperatures [1]. This signature is a vestige of the divergence of this peak in the frictionless-sphere limit [2]. A length scale, defined by the spatial velocity correlation function, and the number hexagons in the Voronoi tessellation have pronounced maxima at the transition. [1] Z. Zhang, D. T. N. Chen, A. G. Yodh, K. B. Aptowicz and P. Habdas, Bull. Am. Phys. Soc. Volume 53, Number 2 (2008). [2] C. S. O’Hern, L. E. Silbert, A. J. Liu and S. R. Nagel, Phys. Rev. E 68, 011306 1-19 (2003).

9:48AM P9.00010 Influence of Confinement on the Structure of Random Close Packing, KENNETH DESMOND, ERIC R. WEEKS, Emory University — We study the structure of many simulated random close packings confined between two walls. Each packing consists of a binary mixture in equal number with a radius ratio of 1.4. Our aim is to quantify how a confining boundary and the thickness between the boundaries alters the structure of randomly close packed disks in 2D and spheres in 3D. We find that confinement lowers the packing fraction, and induces heterogeneity in particle density where particles show strong layering near the wall. Both the particle density and the structure of the local packing show oscillations that decay outward from the wall. The decay in the oscillations is rapid, with a characteristic length scale less than the largest particle diameter. We have also developed a simple model for describing the decrease in packing fraction with confinement.

10:00AM P9.00011 Influence of Confinement on Dynamical Heterogeneities in Dense Colloidal Samples, KAZED EDMOND, ERIC R. WEEKS, Department of Physics, Emory University — We study a colloidal suspension confined between two parallel walls as a model system for glass transitions in confined geometries. The suspension is a mixture of two particle sizes to prevent wall-induced crystallization. We use confocal microscopy to directly observe the motion of the colloidal particles. This motion is slower in confinement, thus producing glassy behavior in a sample which is a liquid in an unconfinned geometry. Like in particles in an unconfined near-glassy system, groups of particles in our confined system move together cooperatively. Normally these groups would be spatially isotropic. However, the confining boundaries induce a layering of the particles. We show that the layering modifies the shapes of the mobile groups within the sample so that they are planar. We investigate how the planar restriction of the shapes of the mobile groups may be the cause of the sample’s glassy behavior.

10:12AM P9.00012 Influence of Boundary Mobility on the Dynamics of Confined Colloidal Suspensions, GARY L. HUNTER, KAZED V. EDMOND, ERIC R. WEEKS, Emory University — We use fast confocal microscopy to study the influence of interfacial mobility and confinement on the dynamics of dense colloidal suspensions. Experiments on confined molecular super-cooled liquids have shown that hard/immobile boundaries result in an increase in relaxation times relative to bulk measurements, whereas soft/mobile boundaries lead to a decrease in relaxation times. We confine suspensions of PMMA microspheres within emulsion droplets of different sizes, thereby probing the consequences of confinement. By changing the viscosity of the external, continuous phase, we also control the interfacial mobility of our samples. In this way, we separate the two effects and draw comparisons between mobility within colloidal suspensions and molecular liquids.

10:24AM P9.00013 Jamming of Foams, GIJS KATGERT, MARTIN VAN HECKE, Kamerlingh Onnes Laboratorium, Universiteit Leiden — We experimentally investigate jamming of soft frictionless spheres at zero stress and zero temperature, using static two-dimensional packings of foam bubbles. As a function of the distance to the jamming point, we obtain the distribution of interparticle forces, the scaling of the contact number and the distribution of free Voronoi area per bubble. Our results compare favorably to earlier predictions for soft discs and grains from theory and numerics.

10:36AM P9.00014 Controlled jamming of particle-laden interfaces using a spinning drop tensiometer, HSIN-LING CHENG, SACHIN VELANKAR, Chemical Engineering, University of Pittsburgh — Partially-wettable particles often adsorb nearly irreversibly at liquid/liquid interfaces. Under conditions when the interface is crowded with a particle monolayer, “2D jamming” can occur, i.e. the interface loses mobility and displays solid-like characteristics. We studied the jamming of iron oxyhydroxide (FeOOH) particles adsorbed at the interface between ethylene glycol and mineral oil using a spinning drop tensiometer (SDT). With decreasing rotational rate, the cylindrical drop retracted due to interfacial tension, and the interface loses mobility and displays solid-like characteristics. We investigated the jamming of iron oxyhydroxide (FeOOH) particles adsorbed at the interface between ethylene glycol and mineral oil using a spinning drop tensiometer (SDT). With decreasing rotational rate, the cylindrical drop retracted due to interfacial tension, and the interface loses mobility and displays solid-like characteristics.

Wednesday, March 18, 2009 8:00AM - 10:48AM – Session P10 FIAP: Focus Session: Multiferroics II

8:00AM P10.00001 Exchange interactions between soft ferromagnetic thin films and multiferroic BiFeO₃, DELPHINE LEBEUGLE, Laboratoire de Physique des Solides, CNRS, Université Paris Sud, 91404 Orsay — Controlling the magnetization of a thin ferromagnetic (FM) film using an electric field is a Holy Grail of nowadays spintronics as it would revolutionize the addressing of magnetic memory elements. One strategy is to combine the magnetoelectric coupling of multiferroic materials like BiFeO₃ (BFO) [1] with the exchange coupling (EC) observed in FM / antiferromagnetic (AFM) systems such as in BFO/CofeB bilayers [2]. BFO is a material of choice as it is one of the very few room-temperature AFM multiferroics. The two types of studied structures consist in FM layers of CoFeB deposited on BFO/STO films as well as thick permalloy layers sputtered onto BFO single crystals. They have been investigated by MagnetOptic Kerr Effect (MOKE) measurements. A macroscopic shift H₀ of the FM loops is a signature of exchange-bias (EB) in bilayers where the FM spins are coupled to the uncompensated AFM ones. We will show that the complex angular dependences of H₀ and Hₑₑ result from the competition between the anisotropies of the FM and AFM layers and the strength of the EC. We will also compare the magnetic properties of the FM layers in relation with the ferroelectric structure of the underlying BFO. In their virgin state, the crystals are in a single ferroelectric and AFM domain with a cycloidal magnetic structure whereas thin films, in which the cyloid is suppressed, are in a highly multidomain state. This comparative study allows us to determine the nature and location of the spins involved in the mechanism of EC. Finally, we present the electric field effect on H₀ and Hₑₑ of these systems. Our previous work on BFO crystals demonstrated that during electrical poling, any change of the polarization direction induces a spin flop of the AFM moments. We will show here that a 90° rotation of the anisotropy axes can be obtained in domains where the polarisation is electrically flipped.

References:


This research has been supported by the Agence Nationale de la Recherche, project “FEMMES” NT05-1 45147.
10:00AM P10.00009 Ideal Nanocheckerboard BiFeO$_3$ – BiMnO$_3$ from First Principles , LUCIA PALOVA, KARIN RABE, PREMALA CHANDRA, Rutgers University — Motivated by recent nanocheckerboard patternings of oxide materials, we use first principles calculations to characterize a prototypical atomic-scale checkerboard of BiFeO$_3$ – BiMnO$_3$ and to compare its properties to those of its bulk constituents. We find this checkerboard has a multiferroic ground state with nonzero ferroelectric polarization and a nonzero magnetic moment, thereby combining desirable features of bulk BiFeO$_3$ and BiMnO$_3$. Unlike either of its parent compounds, structural distortion of the checkerboard stabilizes different magnetic states; this magnetostuctural effect can be used to switch between states with zero and nonzero magnetization. The role of oxygen-octahedron rotations and strain in the magnetic ordering of the nanocheckerboard will be examined in detail.

10:12AM P10.00010 Mechanism of Spontaneous Electric Polarization Flop in TbMnO$_3$ , HAJIME SAGAYAMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, NOBUYUKI ABE, Department of Physics, Tohoku University, TAKA-HISA ARIMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, KAZUAKI IWASA, Department of Physics, Tohoku University — Orthorhombic perovskite TbMnO$_3$ is one of the typical multiferroic systems. Spontaneous electric polarization (P) along the c-axis which originates from the spiral configuration of Mn$^{3+}$ spins rotating in the bc-plane appears below $T_C$ ($\sim 27$K). P/c is turned to the direction along the a-axis by applying a magnetic field along the a-axis. Magnetic structure analysis and a spin-polarized neutron diffraction study of $^{151}$Gd$_{0.02}$Tb$_{0.98}$MnO$_3$ strongly suggest that P/a in TbMnO$_3$ in high magnetic fields also originates from spin spiral rotating in the ab-plane as in the case of P/c. It has been pointed out that anisotropic Tb f-electron magnetic moments play an important role for the complicated electric polarization flop. In this study, we have confirmed the change of spin basal plane of TbMnO$_3$ from the bc- to ab-plane by applying a magnetic field along the b-axis using spin-polarized neutron diffraction technique. We observed that a magnetic fields induce a C-type antiferromagnetic structure caused by the local anisotropy of Tb magnetic moments. We have succeeded in explaining the electric polarization flop of TbMnO$_3$ in terms of a coupling between Mn$^{3+}$ spins and anisotropic Tb magnetic moments.

10:24AM P10.00011 Non-\(d^0\) Mn-driven ferroelectricity in antiferromagnetic BaMnO$_3$ , JAMES RONDINELLI, NICOLA SPALDIN, UC Santa Barbara — Using first-principles density functional theory calculations we predict a ferroelectric ground state structure – driven by off-centering of the magnetic Mn ion – for perovskite-structure BaMnO$_3$. Our finding is surprising, since the competition between energy-lowering covalent bond formation, and energy-raising Coulombic repulsions (the 2nd order Jahn-Teller effect) usually only favors off-centering for non-magnetic $d^0$ ions. It is consistent, however, with the recent observation [S. Bhattacharjee, E. Bousquet and P. Ghosez, Arxiv e-prints 811, 0811.2344 (2008)], that large lattice constants can stabilize polar off-centering of magnetic ions, by lowering the short-range Coulomb repulsions that favor the centrosymmetric phase. We calculate the Born effective charges for the compound, and find anomalously large values for Mn and O, consistent with the large calculated ferroelectric polarization of 30 $\mu$C/cm$^2$. We also describe the changes that occur in the electronic structure when the system transitions from a centrosymmetric to polar state. Finally, we suggest possible routes by which the cubic perovskite phase can be stabilized over the usual hexagonal phase.

10:36AM P10.00012 Antiferromagnetic Resonance in Multiferroic YMnO$_3$ and LuMnO$_3$\(^1\) , SERGEI ZVYAGIN, Dresden High Magnetic Field Laboratory — Multiferroic rare-earth manganeseates have attracted much attention because of the coexistence of ferroelectric and magnetic orders. Combining conventional far-infrared Fourier-transform and THz-range free electron laser electron spin resonance (ESR) spectroscopy techniques, magnetic excitations in hexagonal multiferroic YMnO$_3$ and LuMnO$_3$ in the antiferromagnetically (AFM) ordered phase have been studied. The gap in the excitation spectrum ($\sim 42$ and $\sim 48$ cm$^{-1}$ for YMnO$_3$ and LuMnO$_3$, respectively) was observed directly. Similar slope of the frequency-field dependences of AFM resonance modes, $\sim 0.5$ cm$^{-1}$/T, was revealed for both compounds. A fine structure of AFM resonance absorption has been revealed by means of high-resolution ESR techniques, which can be explained taking into account a finite interaction between the neighboring Mn$^{3+}$ layers. The work was done in collaboration with M. Ozerov, D. Kamensky, E. Čižmár, J. Wosnitza, A.K. Kolezhuk, D. Smirnov, H.D. Zhou, and C.R. Wiebe.

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Wednesday, March 18, 2009 8:00AM - 11:00AM —
Session P11 DCMP: Focus Session: Transport Properties of Nanostructures IV: Correlation Effects

8:00AM P11.00001 Incorporating Exchange-Correlation Effects in Quantum Transport through Nano-scale Junctions , KRISTIAN THYGESEN, Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark — State-of-the-art computational methods for modelling electron transport in nano-scale junctions are based on effective single-particle approximations such as the Kohn-Sham theory of density functional theory. This methodology has been successfully applied to junctions with strong coupling to the metallic electrodes, but has proved insufficient for less homogeneous junctions where the distinction between the nano-device and the electrodes is more pronounced. In order to obtain a more accurate and rigorous description of exchange-correlation effects in weakly correlated molecular junctions, we have implemented the many-body GW approximation within a transport framework suitable to treat non-periodic systems consisting of an interacting region coupled to infinite non-interacting leads with different chemical potentials. Fundamental trends in the properties of metal-molecule-metal junctions are identified on the basis of simple model calculations. These include renormalization of molecular QP levels due to dynamical polarization effects both in- and out of equilibrium as well as the reduction of QP lifetimes due to enhanced QP scattering under finite bias conditions. As will be shown, these genuine many-body effects can have a large influence on the junction IV characteristics even for weakly correlated systems. The importance of using a fully self-consistent GW self-energy for quantum transport calculations will be demonstrated. Finally (preliminary) results for more realistic molecular junctions will be discussed. References: K. S. Thygesen and A. Rubio, PRB 77, 115333 (2008); K. S. Thygesen, PRL 100, 166804 (2008); K. S. Thygesen and A. Rubio, arXiv:0810.5214.

8:36AM P11.00002 ABSTRACT WITHDRAWN —
8:48AM P11.00003 Two-channel Kondo effect and phonon-assisted transport in single-molecular junctions1, LUIS DIAS DA SILVA, ELBIO DAGOTTO, Oak Ridge Natl. Laboratory, Oak Ridge TN, and University of Tennessee, Knoxville TN — The interplay between vibrational modes and Kondo physics is a fundamental aspect of transport properties of correlated molecular conductors. In this theoretical work, we study such interplay in a system consisting of a single molecule in a metallic break junction tuned (by gate voltages) to be in an “odd-N” Coulomb blockade state (Kondo-probe). The connection to left and right metallic leads creates the usual coupling to a conduction channel with left-right symmetry (the “even”-parity channel). A center-of-mass vibrational mode introduces an additional, phonon-assisted tunneling through the asymmetric (“odd”-parity channel). Our numerical renormalization-group calculations reveal that the phonon-mediated coupling to the odd channel leads to the appearance of a two-channel Kondo (2chK) effect, characterized by a non-Fermi-liquid (NFL) fixed point. The ground-state has NFL properties for a critical value of the phonon-mediated coupling strength and critical lines are present for wide range of parameters, including the regime away from particle-hole symmetry. Signatures of this 2chK non-Fermi-liquid behavior are prominent in the thermodynamic properties as well as in the linear conductance.

1Supported by NSF grant DMR-0706020. Research at ORNL is sponsored by DOE-BES under contract DE-AC05-00OR22725.

9:00AM P11.00004 Universal Scaling of Zero-Bias Conductance Peaks in Single-Molecule Transistors Incorporating Tetra[2,3-thiénylene] , ZACHARY KEANE, GAVIN SCOTT, DOUGLAS NATELSON, Rice University — There is significant interest in exploring universal scaling laws as they apply to the Kondo effect in diverse physical systems. One such system is GaAs quantum dots, in which Grobini et al. have demonstrated that the conductance follows a universal scaling function in temperature and source-drain bias. More recently, Scott et al. have demonstrated that the same scaling law applies to single molecule transistors incorporating both C60 and bis(2,5-di-[2]pyridyl-3,4-dithiocyanato-pyrrolate)Cu(II), despite the fact that the relevant energy scales in these systems can differ by 3 orders of magnitude. We will report measurements and universal scaling analysis of the Kondo conductance as a function of temperature and source-drain bias in a fourth system, single molecule transistors incorporating tetra[2,3-thiénylene].

9:12AM P11.00005 Tunneling spectra of individual magnetic endofullerenes molecules , E. S. TAM, J. E. GROSE, J. J. PARKS, B. ULGUT, H. D. ABRUNA, D. C. RALPH, Cornell University, C. TIMM, University of Kansas, M. SCHELOSKE, W. HARNEIT, Freie Universität Berlin — We report measurements of electron tunneling spectra for individual NbC60 molecules, a spin-3/2 endohedral fullerene. The molecules were measured at low temperature in electromigrated break-junctions in the single-electron transistor configuration. We observe that the NbC60 devices exhibit a spin-state transition as a function of applied magnetic field which was not observed in C60 control devices. The nature of this transition enables us to identify the charge and spin states of the molecule. The spectra of NbC60 devices also exhibit low-energy excited states and signatures of non-equilibrium spin excitations predicted for this molecule. The experimental spectra can be reproduced theoretically by accounting for the exchange interaction between the nitrogen spin and electron(s) on the C60 cage.

9:24AM P11.00006 Spin-dependent effects in transport through individual molecules and nanoparticles , J. J. PARKS, E. S. TAM, S. FLORES-TORRES, H. D. ABRUNA, D. C. RALPH, Cornell University — We report measurements of electron transport through individual molecules and nanoparticles incorporated into electromigrated break junction devices. In low-temperature studies of a thiol-terminated organometallic complex using a mechanically controllable break junction, we have studied the effects of molecular distortions. We find that as a function of stretching the molecule, a zero-bias Kondo peak can split into two finite-bias peaks, reminiscent of singlet-triplet transitions in other types of quantum dots. We discuss possible mechanisms in terms of coupling between broken spatial symmetries and the spin state of the molecule. We also measure devices in which molecules and nanoparticles are contacted by ferromagnetic electrodes, so as to study the interplay of spin polarization with single-electron charging effects.

9:36AM P11.00007 Universal Scaling of Nonequilibrium Transport in the Kondo Regime of Single Molecule Devices , GAVIN SCOTT, ZACHARY KEANE, Rice University, Dept of Physics & Astronomy, JACOB CISZEK1, JAMES TOUR, Rice University, Dept of Chemistry, DOUGLAS NATELSON, Rice University, Dept of Physics & Astronomy, Dept of Electrical & Computer Engineering — Scaling laws and universality are often associated with systems exhibiting emergent phenomena possessing a characteristic energy scale. We report nonequilibrium transport measurements on two different types of single-molecule transistor (SMT) devices in the Kondo regime. The conductance at low bias and temperature adheres to a scaling function characterized by two parameters. This result, analogous to that reported recently in semiconductor dots with Kondo temperatures two orders of magnitude lower, demonstrates the universality of this scaling form. We compare the extracted values of the scaling coefficients to previous experimental and theoretical results.

1Current affiliation: Loyola University Chicago, Dept of Chemistry

9:48AM P11.00008 Spatial range of the Kondo effect1, C.A. BÜSSE, G. B. MARTINS, Oakland University, MI, USA, L. COSTA RIBEIRO, E. V. ANDA, PUC-Rio, RJ, Brazil, E. DAGOTTO, University of Tennessee and ORNL, TN, USA — The objective of this work is to discuss the spatial range of the effect caused by the Coulomb interaction localized at an impurity center. The numerical method we use, the embedded cluster approximation (ECA) and the finite U slave boson mean field (FU-SBHF), are developed to treat localized impurity systems. It is important to note that, contrary to other techniques, ECA and FUSB work in real space. Instead of using the spin-spin correlation to determine the length of the Kondo cloud, we will use the local density of states (LDOS) on the lead, far from the impurity. The presence of the impurity produce a disturbance in the LDOS of sites away from it. In this work, we propose to use this distortion to evaluate the spatial range of the Kondo effect. We observe that the effect of the distortion decays exponentially as a function of the distance from the impurity. With that in mind, a characteristic length $L_K$ can be easily defined. When the coupling between the impurity and the metal is increased, we verify that $L_K \sim 1/T_K$. We will also discuss how the magnetic field and temperature affect the length $L_K$.

1We acknowledge the support of NSF grant DMR-0705584

10:00AM P11.00009 1/N expansion of the nonequilibrium single-impurity Anderson Model1, ZURAB RATIANI, ADITI MITRA, New York University — Results are presented for the nonequilibrium single-impurity Anderson model using a large-N approach, where N is the degeneracy of the impurity level. Using the Keldysh formalism, we extend the slave-boson functional integral method of Read and Nussinov to the out of equilibrium current carrying case. The correlation function for the slave boson is shown to exhibit a long time power law behavior along with an exponential decay whose origin is current induced decoherence, a result consistent with nonequilibrium X-ray edge physics. Expressions for the impurity susceptibility and the conductance through the device are presented to $O(1/N)$ and for an applied voltage less than the Kondo temperature.

1Supported by NSF-DMR 0705584
demonstrated the expected suppression of shot noise when junction conductance is near an integer multiple of the conductance quantum, $G$. Previous experiments at low temperatures in metal and semiconductor point contacts have approach is illustrated on several two-terminal nanostructures. I will also discuss the relationship between the present approach and the Landauer-Büttiker model that averages over transmission coefficients. Full understanding of RSOI on the Kondo regime is fundamental, as it studies the competition of different coherent phenomena and has potential applications in devices such as spin-filters. A study of this geometry included the role of RSOI perturbatively [1]. However, the full features of Kondo physics are subtle and not captured in perturbation theory. In this work, we present a numerical renormalization group study that addresses charge and spin transport properties in the zero-bias regime, and allows comparisons with perturbation results. We find that the presence of both AB fields and RSOI results in an intrinsic polarization field that breaks the spin degeneracy. This allows a delicate control of spin polarization of the conductance in the system, while strong RSOI suppresses the Kondo effect. [1] R. J. Heany et al., PRB 77, 155132 (2008)

Supported by NSF-DMR MWN grant 0710581.

Decoherence due to contacts in ballistic nanostructures[1]. I. KNEZEVIC, University of Wisconsin - Madison — In quasiballistic nanoscale electronic structures, the process of relaxation towards a steady state cannot be attributed to carrier scattering. Rather, the active region of a nanostructure is an open quantum-mechanical system, whose nonunitary evolution (decoherence) toward a nonequilibrium steady state is determined by carrier injection from the rapidly dephasing contacts. I will present a technique for the treatment of contact-induced decoherence in ballistic nanostructures, which is established within the framework of the open system theory. Efficient electron-electron scattering in the contacts enables one to consider them nearly “memoryless” and derive a Markovian kinetic equation for the active region’s statistical operator through coarse graining over the contacts’ short memory-retention time. By incorporating a first-principles model interaction between the active region and the contacts into the Markovian dynamics derived, nonequilibrium steady-state distribution functions of the forward- and backward-propagating states in the active region are derived analytically. The approach is illustrated on several two-terminal nanostructures. I will also discuss the relationship between the present approach and the Landauer-Büttiker formalism, as well as the inclusion of scattering.

Supported by the NSF, award ECCS-0547415.

High frequency measurements of shot noise suppression in atomic-scale metal contacts[1]. PATRICK J. WHEELER, Department of Physics and Astronomy, Rice University, KENNETH EVANS, Applied Physics Program, Rice University, JEFFREY RUSSOM, Department of Physics and Astronomy, Rice University, NICHOLAS KING, Department of Physics and Astronomy, DOUGLAS NATelson, Department of Physics and Astronomy, Rice University — Shot noise provides a means of assessing the number and transmission coefficients of transmitting channels in atomic- and molecular-scale junctions. Previous experiments at low temperatures in metal and semiconductor point contacts have demonstrated the expected suppression of shot noise when junction conductance is near an integer multiple of the conductance quantum, $G_0 \equiv 2e^2/h$. Using high frequency techniques, we demonstrate the high speed acquisition of such data at room temperature in mechanical break junctions. In clean Au contacts conductance histograms with clear peaks at $G_0$, 2$G_0$, and 3$G_0$ are acquired within hours, and histograms of simultaneous measurements of the shot noise show clear suppression at those conductance values. We describe the dependence of the noise on bias voltage and analyze the noise vs. conductance histograms in terms of a model that averages over transmission coefficients.

The authors acknowledge support of the Robert A. Welch Foundation grant C-1636 and NSF DMR-0347253.

Wednesday, March 18, 2009 8:00AM - 11:00AM – Session P12 DMP DCMP: Focus Session: Characterization and Modeling of Complex Surfaces and Interfaces 308

Atomistic Structure and Energy of Solid-Liquid Interfaces, WAYNE KAPLAN, Technion - Israel Institute of Technology — As microstructural length-scales are reduced, the role of interfaces in determining the properties of materials becomes more dominant. The importance of the correlation between interface structure and chemistry with interface (and bulk) properties is evident in a range of material systems, and is a topic of intense experimental and theoretical work for solid-solid interfaces. While detailed thermodynamic analysis of solid-liquid interfaces is routinely conducted, knowledge of the local structure at solid-liquid interfaces is still incomplete. To be more specific, the correlation between the structure of the solid, and the structure in the liquid near the interface, has not been fully addressed. In this presentation, in-situ (~750 °C) high resolution transmission electron microscopy (HRTEM) of liquid Al in contact with sapphire ($\alpha$-Al$_2$O$_3$) will be presented. Contrast perturbations in the liquid Al adjacent to the crystalline substrate were determined to be due to ordering of the liquid, via detailed multi-slice dynamic electron scattering simulations. Details on the type of ordering were interpreted by molecular dynamics simulations of liquid Al in contact with crystalline substrates, and compared to sessile drop studies of liquid Al on sapphire. These results are compared with recent HRTEM investigations of equilibrium amorphous films at metal-Al$_2$O$_3$ interfaces, where partial ordering of the film plays an important entropic role in reaching stable nanometer-thick films. This will then be extended to equilibrium segregation, and the concept of extremely small volumes of liquids confined by crystals.
8:36AM P12.00002 Calculation of excess interfacial entropy, stress and energy for solid-liquid interfaces

BRIAN B. LAIRD, Dept. of Chemistry, Univ. of Kansas, RUSLAN L. DAVIDCHACK, Dept. of Mathematics, Univ. of Leicester, UK, MARK ASTA, YANG YANG, Dept. of Chem. Eng. and Materials Sci., UC Davis — The solid-liquid interfacial free energy, \( \gamma_{\text{sl}} \), governs a number of important phenomena, e.g., crystal nucleation and growth, and wetting. For an equilibrium crystal-melt interface, \( \gamma_{\text{sl}} \) can be calculated via simulation using thermodynamic integration or capillary fluctuations [Phys. Chem. B 109, 17802 (2005)]. The calculation of \( \gamma_{\text{sl}} \) away from coexistence requires the temperature and strain dependence of \( \gamma_{\text{sl}} \), which can be determined from the excess interfacial entropy, \( \eta_{\text{sl}} \), and stress tensor, \( \tau_{\text{sl}} \). We determine \( \eta_{\text{sl}} \) and \( \tau_{\text{sl}} \) for a system of Lennard-Jones particles and for particles with an inverse-power interaction \( [\phi(r) = \epsilon / r^n] \) for \( n = 6, 8 \) (fcc and bcc) and 12, 20 (fcc). We determine \( \eta_{\text{sl}} \) and \( \tau_{\text{sl}} \) for the (100), (110) and (111) orientations. We calculate \( \eta_{\text{sl}} \) using two methods, both using the Gibbs dividing surface defined so that the excess interfacial particle number is zero. In the first, we calculate \( \eta_{\text{sl}} \) from the temperature dependence of \( \gamma_{\text{sl}} \), \( \tau_{\text{sl}} \) and the number density, \( \rho \), along the coexistence curve. In the second, we calculate the excess interfacial energy, \( \eta_{\text{sl}} \), and use the equation \( \gamma_{\text{sl}} = \epsilon_{\text{sl}} - T \eta_{\text{sl}} \). The results agree within estimated errors. One surprising observation is that \( \eta_{\text{sl}}, \epsilon_{\text{sl}} \) and \( \tau_{\text{sl}} \) are significantly more anisotropic than \( \gamma_{\text{sl}} \).

8:48AM P12.00003 Spin Order in Magnetic Organic Semiconductor V[TCNE]∼2

HAILEMARIAM AMBAYE, VALERIA LAUTER, STEPHEN NAGLER, CHRISTINA HOFFMANN, Ornlé, HAL LÉE, ANDREW PÄZNT, Ornlé, ARTHUR ÉPSTEIN, CHEN CHI-YI, Ohio state university, RICHARD GÓYETTE, Ornlé — These Organic-based magnets are new area of materials research. The discovery of V[TCNE]∼2 with its high Tc ∼ 400 K and semiconducting behavior similar to silicon, as well as its photonic response unique for magnetic materials, opens up many issues of fundamental physics and chemistry as well as the potential opportunities for use of these and related materials in technologies ranging from spintronics to sensing. To understand the magnetic state and the evolution of the magnetic at and near interfaces with other magnetic and non magnetic materials we have performed a polarized neutron measurement at the SNS magnetism reflectometer instrument. The measurements show the presence of magnetic resonances at 5K temperature. The room temperature measurements show no magnetic responses. The systems considered are magnetic and non magnetic materials we have performed a polarized neutron measurement at the SNS magnetism reflectometer instrument. The measurements show the presence of magnetic resonances at 5K temperature. The room temperature measurements show no magnetic responses. The systems considered are V[TCNE]∼2(1500A) and 6000A on Si substrate. Work supported by DOE.

9:00AM P12.00004 Stabilization of a ferromagnetic insulating phase with colloidal magnetore sistance at the interface of manganese bilayers

JONATHAN LAVERDIÈRE, SERGE JANDL, PATRICK FOURNIER, Université de Sherbrooke — The charge ordered phase observed in colloidal magnetoresistive mangetites motivated many theoretical and experimental efforts. Charge order is an insulating electronic phase that becomes metallic in sufficiently high magnetic field. This high “milling” field hinders any applications for magnetic storage devices. Here, we present the study of the proximity effect in Nd$_{0.57}$Sr$_{0.13}$MnO$_3$ (NSMO) / Nd$_{0.55}$Ca$_{0.15}$MnO$_3$ (NCMO) bilayers. NSMO is dominated by ferromagnetic double exchange, producing a ferromagnetic metallic phase, while NCMO is strongly influenced by the Jahn-Teller lattice distortion, localization charges on the Mn$^{3+}$ sites. Our study addresses the following question: Which one will dominate at the NSMO/NCMO interface? We will present Raman scattering and magnetotransport measurements on NCMO/NSMO bilayers grown on SrTiO$_3$ substrate. A ferromagnetic insulating phase has been observed for very thin NSMO films. This phase becomes metallic and gives rise to colossal magnetoresistance at a low field compared to the usual melting field.

9:12AM P12.00005 Effects of surfactant on the physical properties of single-walled carbon nanotube buckypaper.

JIN GYU PARK, CHARLIE LIN, JESSE SMITHYMAN, ADAM COOKE, SHU LI, RICHARD LIANG, CHUCK ZHANG, BEN WANG, High-Performance Materials Institute, Florida State University, ADE KIYARAHARJDJA, JAMES BROOKS, Department of Physics, Florida State University, HIGH-PERFORMANCE MATERIALS INSTITUTE, FLORIDA STATE UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, FLORIDA STATE UNIVERSITY COLLABORATION, BANDGAP ENGINEERING INC. COLLABORATION, DEPARTMENT OF PHYSICS AND DEPARTMENT OF ELECTRICAL ENGINEERING, MIT COLLABORATION — Bulk bismuth has a small band overlap between the conduction and valence bands and a highly anisotropic electron effective-mass tensor. Previously, we have shown evidence for strong quantum confinement in Bi nanorods with diameters ~10 nm which undergo a transition from a semimetal with a small band overlap to a semiconductor with a small indirect band gap. These quantum confinement effects can be potentially useful in optical and electro-optical devices. Here, we report the low temperature (77 K) optical absorption properties of ~10 nm diameter Bi nanorods using Fourier Transform Infrared spectroscopy. The Bi nanorods exhibit a strong absorption peak (~1000 – 1400 cm$^{-1}$, depending on the diameter) in the mid-IR that is not present in bulk bismuth. The full width at half maximum intensity of the IR absorption peaks decrease from 26 cm$^{-1}$ at 300 K to 15 cm$^{-1}$ at 77 K. No significant blue-shift in energy was observed, and these changes will be discussed in terms of the temperature dependence of the L-point and T-point electron energies.

9:24AM P12.00006 Low-Temperature Absorption Studies in Bismuth Nanowires

JASON REPPERT, Clemson University, MALCOLM SKOVE, MARCIE BLACK, MILDRED DRESSELHAUS, APPARAO RAO, SCHOOL OF MATERIALS SCIENCE AND ENGINEERING, CLEMSON UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS AND ASTRONOMY, COMSET, CLEMSON UNIVERSITY COLLABORATION, BANDGAP ENGINEERING INC. COLLABORATION, DEPARTMENT OF PHYSICS AND DEPARTMENT OF ELECTRICAL ENGINEERING, MIT COLLABORATION — Bulk bismuth has a small band overlap between the conduction and valence bands and a highly anisotropic electron effective-mass tensor. Previously, we have shown evidence for strong quantum confinement in Bi nanorods with diameters ~10 nm which undergo a transition from a semimetal with a small band overlap to a semiconductor with a small indirect band gap. These quantum confinement effects can be potentially useful in optical and electro-optical devices. Here, we report the low temperature (77 K) optical absorption properties of ~10 nm diameter Bi nanorods using Fourier Transform Infrared spectroscopy. The Bi nanorods exhibit a strong absorption peak (~1000 – 1400 cm$^{-1}$, depending on the diameter) in the mid-IR that is not present in bulk bismuth. The full width at half maximum intensity of the IR absorption peaks decrease from 26 cm$^{-1}$ at 300 K to 15 cm$^{-1}$ at 77 K. No significant blue-shift in energy was observed, and these changes will be discussed in terms of the temperature dependence of the L-point and T-point electron energies.

9:36AM P12.00007 Nanopatterned Biomimetic Surfaces to Promote the Role of Cytoskeletal Proteins in Cell Adhesion

JUSTIN ABRAMSON, MATTEO PALMA, Department of Mechanical Engineering, Columbia University, MARK SCHWARTZMAN, Department of Chemical Engineering, Columbia University, SHALOM WIND, Department of Applied Physics and Applied Mathematics, Columbia University, MICHAEL SHEETZ, Department of Biological Sciences, Columbia university, JAMES HONE, Department of Mechanical Engineering, Columbia University — Nanometer level spatial organization has been shown to play a crucial role in cell mechanics, in particular in cell adhesion to the extracellular matrix. Combining nanolithography and biomolecular self-assembly strategies, we report on the fabrication of nanopatterned biomimetic surfaces to probe the importance of both the spatial ordering of transmembrane proteins as well as the role played by peptide sequences as cell binding domains in the formation of cell focal adhesions. We have fabricated arrays of Au/Pd nano-dots using electron-beam and nanoimprint lithography. Different chemical strategies have been pursued to biofunctionalize such nanostructures, both through the formation of mixed Self Assembled Monolayers as well as via chemical reactions at surfaces. Fluorescence microscopy allowed us to monitor single-molecule chemisorption of cell-adhesion proteins in vitro, as well as to follow cell spreading on the nanopatterned bio-arrays, in order to investigate cytoskeletal protein binding interactions in vivo.

1Work supported by CIFAR, CFI, NSERC (Canada) and FQRNT (Québec).

2This research was supported by AFOSR and AFRL.
9:48AM P12.00008 Molecular Dynamics Simulations of Interfaces in Complex Materials. TAHIR CAGIN, Texas A&M University — Molecular details of structure and chemistry play an important role in the properties and engineering performance of composites and complex materials. Experimental investigation of the interfaces most often presents itself as a major challenge. This, in turn, becomes an opportunity in disguise for the molecular level simulation approaches. However, in order to convincingly address to the problem of elucidating the structure and chemistry at the interfaces, one must employ reliable and accurate and transferable interaction potentials for dissimilar materials - this is the case for composites and complex materials. In this talk, we will present examples of molecular dynamics studies on the structure and properties of silicon nano-crystals in a silica matrix, piezoelectric CNT-polyimide nano-composites, and on the role of super lattice structures for enhancing mechano-electric coupling in ferro-electric ceramic alloys.

10:24AM P12.00009 Evaluation of dispersion interactions in general geometries. ANTHONY MAGGS, CNRS-ESPCI, PASQUALI SAMUELA, IBPC-Paris 7 — Dispersion interactions are very often approximated by pairwise van der Waals interactions between molecules. In dense media, however, there are important corrections due to the many-body nature of fluctuations. These many-body forms can be calculated in closed form in the simplest of geometries using the methods of Casimir and Lifshitz. Here we study dispersion interactions between bodies in general geometries. We map the calculation of the partition function onto a determinant which we discretize and evaluate with the help of Cholesky factorization. We study the efficiency of the factorization in two and in three dimensions and conclude that accuracies of the order of one per cent are readily achieved in the total interaction energy. We compare the approximations of pairwise additivity and proximity force with our numerical methods.

10:36AM P12.00010 Phase-field Simulation of Phase Coarsening at Ultra-high Volume Fractions. KE-GANG WANG, XUERU DING, Department of Physics and Space Sciences, Florida Institute of Technology, Melbourne, FL 32901 — The study of phase coarsening kinetics during microstructure evolution is critical to a variety of industrial applications involving two-phase systems in which the dispersed phase controls the properties of the material. Liquid-phase sintering, casting and spray deposition are just a few examples of processes in which the coarsening process has important technological implications. In this talk, the dynamics of phase coarsening at ultra-high volume fractions (V_c > 0.9) will be presented based on 2-D phase-field simulations. Kinetics of phase coarsening and spatial correlations in microstructures will be revealed. Pair distribution functions in microstructures will be shown. The scaled particle-size distribution as functions of the dispersed volume fraction will be demonstrated. Finally, computational results are compared with experimental observations.

10:48AM P12.00011 The impact of self-healing on the life-time of materials. JOHN GADDY, WOUTER MONTFROOIJ, University of Missouri, ALEXANDER SCHMETS, Delft University of Technology — Structural materials that are attributed with the (new) property of "self-healing" will obviously lead to safer, longer lasting and more reliable structures. The property of "self-healing" can be defined as the ability of a material to mitigate autonomously early stages of damage such as micro cracks, and many examples of materials with this properties have been reported in recent years [1]. In this contribution we investigate the effect of healing on the expected service life time of a model material. We apply a statistical mechanics' inspired computational approach to model the process of damage accumulation and on-site healing of a material under well defined loading conditions. We define a material as being at the end of its service life when a percolative path of damaged cells has passed a prescribed length. The variation of service life for various scenarios, such as healing times and distribution of healing centers is investigated. Finally we show how this type of models may be useful for the design of optimized self-healing materials.


Wednesday, March 18, 2009 8:00AM - 11:00AM —
Session P13 DCOMP GSCCM: Focus Session: Extreme Conditions and High Pressure I: Chemistry

8:00AM P13.00001 Shock-induced Reactions in Pentaerythritol Tetranitrate Studied by Molecular Dynamics Simulation 1. JOANNE BUDZIEN, AIDAN P. THOMPSON, Sandia National Laboratories, SERGEY V. ZYBIN, California Institute of Technology — Molecular dynamics simulations were performed using the reactive force field, ReaxFF, as implemented in the General Reactive Atomistic Simulation Program code for systems consisting of a single crystal of PETN with not fewer than 237000 atoms. The crystals were shocked along the [100] direction using two different piston velocities. The resulting chemical reactions were tracked in an attempt to elucidate short-time initiation mechanisms. Here, we present the primary, secondary, and intermediate products as a function of time and position behind the shock front.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

8:12AM P13.00002 Molecular dynamics simulations of uniaxial shock compression of RDX crystals. DMITRY BEDROV, JUSTIN HOOKER, GRANT SMITH, University of Utah — Using the Hugoniot method atomistic molecular dynamics simulations of uniaxial shock compressions along [001], [100], and [010] directions of RDX crystal have been conducted over a wide range of shock pressures. The Hugoniot simulations allow modeling of shocked material without the necessity to have extremely large simulation cell required to explicitly resolve the shock wave propagation. Hugoniot simulations on systems containing only few thousand molecules allowed us to determine Hugoniot elastic limit and to investigate shock-induced shear banding and phase transition in RDX crystal.

8:24AM P13.00003 A molecular dynamics study of the role of pressure on the response of reactive materials to thermal initiation. N. SCOTT WEINGARTEN, WILLIAM D. MATTSON, BETSY M. RICE, U. S. Army Research Laboratory, ANTHONY D. YAU, High Performance Technologies, Inc., TIMOTHY P. WEIHS, Johns Hopkins University — Reactive materials have the potential for implementation into a wide variety of commercial and military applications. However, the fundamental physical and chemical processes that control the energy release are not well understood. To elucidate the mechanisms of energy release, we simulated the exothermic alloying reactions of a Ni/Al bilayer with initial temperatures of 1100 K and 1500 K using both microcanonical (NVE) and isoentropic (NPH) molecular dynamics simulations with an embedded atom method (EAM) potential. The mechanism of the mixing is the same for all simulations: as mixing and reaction occurs at the interface, the heat generated first melts the Al layer, and subsequent mixing leads to further heat generation after which the Ni layer melts, leading to additional mixing until the alloying reactions are completed. The results indicate that pressure has a significant influence on the rates of atomic mixing and alloying reactions. In addition, two-phase coexistence simulations were used to determine the melting temperatures of pure Al and pure Ni at various pressures using this potential, and these values are discussed within the context of the Ni/Al bilayer results.
8:36AM P13.00004 Mbar Chemistry: Novel States of Matter in Extreme Conditions

SHIK YOO, Department of Chemistry and Institute for Shock Physics, Washington State University, Pullman, Washington 99164-2816 USA — Compression energy at 100 GPa often exceed several eV/atom, rivaling the energy of strong chemical bonds. Therefore, the application of such a high pressure significantly alters the chemical, electronic/optical, thermomechanical properties of solids and, in turn, provides a way to test condensed matter theory and to exploit novel materials with advanced properties. Furthermore, recent advances in diamond-anvil cell high-pressure technologies coupled with advanced third-generation synchrotron x-ray offer unprecedented opportunities to discover exotic states of matter at high pressure-temperature conditions of the Earth and planetary interiors. In this paper, I will discuss several recent results of high-pressure chemistries that occur in simple low Z molecular solids to novel nonmolecular extended solids. Broadly speaking, these molecular-to-nonmolecular transitions occur as a result of the pressure-induced electron delocalization arising from a rapid increase in electron kinetic energy at high density. Yet, the details are substantially more complicated because of the phase metastability, large lattice strain, and governing kinetics. As a result, there are many outstanding questions regarding the exact nature of chemical bonding, phase stability, and transition mechanisms. Also, presented are several future directions of high pressure materials research in an complementary phase and time scales of dynamic and static high pressures.

9:12AM P13.00005 Novel Catalytic Behavior of Dense Hot Water in PETN Decomposition Reactions

CHRISTINE WU, LAURENCE FRIED, LIN YANG, NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore National Lab — Under extreme conditions, water is known to exhibit fascinating physical behaviors. Its remarkable structural and phase complexity strongly suggests that its chemical properties may be unusual as well, which have remained largely unrevealed. Using ab initio molecular dynamics simulations, we have recently discovered that water plays a non-trivial role in catalyzing complex reactions of a high explosive pentaerythritol tetranitrate (PETN). This finding is in contrary to the current view of water as a stable final product of high explosive reactions, and has possible implications in geochemistry, such as reactions in planetary interiors.

This work preformed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:24AM P13.00006 The formation of carbon nitride clusters in shocked insensitive explosives

LAURENCE FRIED, RIAD MANAA, EVAN REED, NIR GOLDMAN, Lawrence Livermore National Laboratory — Many high explosives are organic molecular crystals that contain both oxidizing and reducing functional groups. These solids rapidly release their energy in supersonic detonation waves. It has been observed that explosives rich in carbon tend to have much longer reaction zones than those that do not. These explosives form graphitic or diamond-like carbon particles during detonation. The slow diffusion-limited process of forming the solid carbon from bulk explosives is believed to a play a central role in determining the reaction zone length of a given explosive. In this work, we identify an altogether new mechanism for the slow reactvity of carbon rich explosives. Quantum-based multi-scale simulations of shocked 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) provide the first evidence for the formation of nitrogen-rich heterocyclic clusters that impede the formation of fluid nitrogen and solid carbon.

This work was performed by the Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

9:36AM P13.00007 Ab initio molecular dynamics of hypervelocity chemistry

IGOR SCHWEIGERT, BRETT DUNLAP, Theoretical Chemistry Section, US Naval Research Laboratory, 4555 Overlook Ave SW, Washington, DC 20375 — Resolving chemical dynamics of decomposition of energetic molecules is crucial for understanding detonation initiation in energetic materials and predicting their sensitivity to shock and impact stimuli. We employ Born-Oppenheimer molecular dynamics driven by density-functional methods to identify possible decomposition pathways in nitric esters (including pentaerythritol tetranitrate) and to understand the effect of collision orientation and velocity. Studies of the potential energy surface in the bond-breaking region, unimolecular decomposition, and binary hypervelocity collisions of model nitric esters (methyl and ethyl nitrates) will be reported. Methodological challenges in describing extensive changes in the electronic structure that accompany decomposition will be discussed.

This work was supported by the Naval Research Laboratory via the National Research Council of the National Academy of Science and by the Office of Naval Research, both directly and through the Naval Research Laboratory.

9:48AM P13.00008 Boron carbides from first principles

EMMANUEL BETRANHANDY, JELENA SJAKSTE, NATHALIE VAST, Laboratoire des solides irride d’École polytechnique-CEA-CNRS — In this work, we focus on the understanding gained from the investigation of the physical properties of boron-carbides with theoretical methods based on density functional theory (DFT). Comparison of computed and experimental vibrational or NMR spectra has shown that the atomic structure of B$_4$C consists in C-B-C chains linking mostly B$_3$Cicosahedra, and a few percent of B$_2$C$_2$icosahedra. In particular, C-C-C chains are excluded and can not be responsible for B$_4$C amorphization under shockwaves. In this work we find that at lower carbon concentration all models are metastable with respect to B$_3$C plus α-boron. This could explain actual difficulties in the synthesis of clean samples. Furthermore we discuss effects of temperature and/or pressure on stabilities and properties. Finally, the idea of combining high hardness and superconductivity in the same material by doping boron-rich solids has emerged. We show results on the strength of the electron-phonon coupling constant obtained with DFT-based methods in B$_3$C$_2$.

Support from DGA through a grant is gratefully acknowledged. Results have been obtained in part with the espresso package and computer time granted by CEA DSM on the NEC SX8.

10:00AM P13.00009 Dynamical stability of the cubic metallic phase of AlH$_3$ at ambient pressure

DUCK YOUNG KIM, RALPH H. SCHEICHER, Condensed Matter Theory Group, Department of Physics and Materials Science, Uppsala University, Box 530, SE-751 21, Uppsala Sweden, RAJEEV AHUJA, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm — We have characterized the high-pressure cubic phase of AlH$_3$ using density functional theory to determine mechanical as well as electronic properties and lattice dynamics from the response function method [1]. Metallization in AlH$_3$ under pressure has been studied, which is of great interest not only from a fundamental physics point of view for the study of phenomena related to metallic hydrogen, but also, because metallic AlH$_3$ possesses weaker Al-H bonds than other insulating phases [2]. Our phonon calculations show the softening of a particular mode with decreasing pressure, indicating the onset of a dynamical instability that continues to persist at ambient conditions. We find from analyzing the atomic and electronic interactions using theoretical calculations that finite-temperature effects lead to the desired stabilization of metallic AlH$_3$ at ambient conditions.

The simulations are performed using the Multi-Scale Shock Method (MSST) which we have extended to maintain thermodynamic equilibrium between electrons and ions to correctly treat electronic heat capacity.

This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
9:00AM P14.00006 Colloidal Hydrodynamics with Arbitrary Boundary Conditions. JONATHAN K. WHITMER, ERIK LUIJTEN, University of Illinois at Urbana-Champaign — Hydrodynamic interactions are essential to the understanding of colloidal dynamics. Due to their complexity and computational cost, they are often ignored in simulations. Over the past decade, coarse-grained methods such as Stochastic Rotation Dynamics (an example of the larger family of Multi-Particle Collision (MPC) methods) have been developed to include these interactions efficiently in simulation. To use these methods for the study of self-assembly dynamics of particles with anisotropic surface chemistry, we extend previously implemented methods for stick boundary conditions to arbitrarily slipping surfaces on the curved surfaces of spherical colloids. We present a mapping from an easily tunable simulation parameter onto the slip length as defined by Navier, and discuss the dynamics of anisotropic particles simulated using this method.


9:12AM P14.00007 Reversible Rayleigh-to-Mie Scattering Transition in a Core-Shell Colloidal System. GUANGNAN MENG, Harvard University, ADELINE PERRO, VINOTHAN MANOHARAN — We present a study of light scattering from colloidal particles with small polystyrene cores and large shells of poly(N-isopropylacrylamide-co-acrylic acid). When swollen in deionize water at room temperature, the shell is nearly index-matched to pure water, and the scattering is dominated by Rayleigh scattering from the polystyrene cores. As we change the solvent condition by increasing temperature or salt concentration, the shell starts to shrink and scatter light. Both the scattering cross section and the forward scattering of the particles increase, characteristic of Mie scatterers. We use optical microscopy, static light scattering and turbidimetry to study this optical transition. Such core-shell particles might be used as aqueous index-matched tracer colloids, as model scatterers for self-assembly studies, or as optical filters with tunable opacity.

9:24AM P14.00008 Pressure driven foam flow rheology. C.D. JONES, K. NORDSTROM, D.J. DURIAN, University of Pennsylvania — We probe the complex rheology of 3d foams by flowing them through a narrow column. The foam flows upward through one of two vertical rectangular columns with a 41 cross-sectional aspect ratio, by bubbling gas through a soapy solution at the base of our apparatus. One column is clear acrylic sheet on all sides, which is slippery to the foam, and results in plug flow. The other column has the narrow surfaces covered with sandpaper, giving them a sticky surface, which creates shear due to the zero velocity boundary condition. As expected, the flow profile between the slippery broad faces is flat, however the profile between the narrow, sticky faces exhibits a curved velocity profile that is strongly dependent on flow rate. We are able to analyze a 2d velocity profile from a 3d bulk system, whereas other recent foam rheology work has been constrained to the 2d system. We employ particle image velocimetry to measure the strain rate, and compute the stress from the pressure drop along the channel, to investigate the local stress-strain relationships in a flowing foam.

1Supported by DOE Office of Basic Energy Sciences, grant DE-FG02-06ER46298

9:36AM P14.00009 Effective temperature of a sheared foam. DANIEL VALDEZ-BALDERAS, University of Rochester, PETER OLSSON, Umea University, STEPHEN TEITEL, University of Rochester — We perform computer simulations of a model for an overdamped, sheared foam in two dimensions at zero temperature. We measure an effective temperature with the use of an embedded oscillator, in manner analogous to experiments done by Abate and Durian on a different system [arXiv:0806.0765v2]. Our oscillator is one of the bubbles in the foam, which, in addition to its interaction with other bubbles, is also subject to a harmonic potential. We define an effective temperature based on the fluctuations in the position of the oscillator. We compare our results to the effective temperatures computed with the use of measurements of the fluctuations of the shear stress and fluctuations of the energy, respectively.

9:48AM P14.00010 Realization spaces of bubble clusters and coarsening trajectories. BRYAN CHEN, RANDALL KAMIEN, University of Pennsylvania — In the search for a more unified description of the geometry of equilibrium foams, we study the space of all realizations of equilibrium bubble clusters of fixed topology. The geometry of foam is highly constrained due to the area minimization property - in two dimensions, this means that all interfaces must be portions of circles and interfaces intersect in threes at angles of 120°. This results in a finite dimensional space of bubble clusters, and the dynamics of coarsening via gas diffusion induces a vector flow on it. The boundaries and singularities of the realization space may be identified with topological transitions and instabilities in coarsening.

10:00AM P14.00011 Experimental studies of low-density fluid phases in tunable dipolar colloids. ANAND YETHIRAJ, NING LI, HUGH NEWMAN, MANUEL VALERA, IVAN SAIKA-VOIVOD, Memorial University — Experiments of low-density colloidal fluid phases in the presence of an external electric field are presented. We obtain angular order parameters as a function of the applied electric field. When plotted against a dimensionless dipole strength parameter, the order parameters for different particle sizes fall on a single curve, suggesting that colloids in a fluid phase in the presence of electric fields do indeed interact by an effective point dipolar interaction. We then explore the statistics of particle packings at low-density and extract the experimental compressibilities and equation of state for these dipolar colloids.

1This work is being supported by NSERC
2(present address: Brandeis University)
3(present address: Slippery Rock University)

Wednesday, March 18, 2009 8:00AM - 11:00AM – Session P15 DFD: Biologically Inspired Physics: Swimming, Propulsion, Bio-fluids 316

8:00AM P15.00001 Swimming in a vortex street. SILAS ALBEN, Georgia Tech — Recent studies showed that a trout swimming in a cylinder wake can save energy by “slaloming” through a vortex street. We present a simple model using a flexible body with vortex sheets, and find swimming shapes which maximize output power and efficiency. We find analytic solutions and compare the optimal swimming phase between the body and vortices with previous experiments and numerics.

1NSF-DMS support is acknowledged.

8:24AM P15.00003 Collective locomotion of non-swimmers, ERIC LAUGA, University of California, San Diego (USA), DENIS BARTOLO, ESPCI (France) — To achieve propulsion at low Reynolds numbers, a swimmer (e.g. a biological cell such as a bacterium, or a spermatozoon) must deform its shape in time in a way that is not invariant under time-reversal symmetry (non-reciprocal); this is Purcell’s scallop theorem. We show here explicitly that there is no many-scallop theorem. Two active bodies undergoing reciprocal deformations - and therefore incapable of swimming when considered separately - can exploit hydrodynamic interaction to swim. If the bodies are polar, we also show that they experience effective long-range interactions. We derive our results analytically for a minimal dimers model, and generalize them to more complex geometries on the basis of symmetry and scaling arguments. Furthermore, we explain how such cooperative locomotion can be realized experimentally by shaking a collection of soft particles with a homogeneous external field, thereby making non-swimmers swim.

8:36AM P15.00004 Self-Assembled Magnetic Surface Swimmers: Theoretical Model†, IGOR ARANSON, MAXIM BELKIN, ALEXEY SNEZHKO, Argonne National Laboratory — The mechanisms of self-propulsion of living microorganisms are a fascinating phenomenon attracting enormous attention in the physics community. A new type of self-assembled micro-swimmers, magnetic snakes, is an excellent tool to model locomotion in a simple table-top experiment. The snakes self-assemble from a dispersion of magnetic microparticles suspended on the liquid-air interface and subjected to an alternating magnetic field. Formation and dynamics of these swimmers are captured in the framework of theoretical model coupling paradigm equation for the amplitude of surface waves, conservation law for the density of particles, and the Navier-Stokes equation for hydrodynamic flows. The results of continuum modeling are supported by hybrid molecular dynamics simulations of magnetic particles floating on the surface of fluid.

8:48AM P15.00005 Accumulation of microswimmers near surface due to steric confinement and rotational Brownian motion, GUANGLAI LI, JAY TANG, Brown University — Microscopic swimmers display some intriguing features dictated by Brownian motion, low Reynolds number fluid mechanics, and boundary confinement. We re-examine the reported accumulation of swimming bacteria or bull spermatozoa near the boundaries of a fluid chamber, and propose a kinetic model to explain how collision with surface, confinement and rotational Brownian motion give rise to the accumulation of micro-swimmers near a surface. In this model, an elongated microswimmer invariably travels parallel to the surface after hitting it from any incident angle. It then takes off and swims away from the surface after some time due to rotational Brownian motion. Based on this analysis, we obtain through computer simulation steady state density distributions that reproduce the ones measured for the small bacteria E coli and Caulobacter crescentus as well as for the much larger bull spermatozoa swimming near surfaces. These results suggest strongly that Brownian dynamics and surface confinement are the dominant factors for the accumulation of microswimmers near a surface.

9:00AM P15.00006 Modeling the Behavior of Self-Propelled Microcapsules, AMITABH BHATTACHARYA, Dept of Chemical Engg, University of Pittsburgh, O. BERK USTA, ANNA C. BALAZS, Dept of Chemical Engg, Univ Pittsburgh — Biological cells can perform complex tasks by signaling and moving autonomously in their environment. We study a system of self-propelled microcapsules, first proposed by Usta et al (2008), that mimics this process. It consists of a signaling and target microcapsule placed close to an adhesive substrate and immersed in fluid. The signaling microcapsule encases nanoparticles, which, when released, modifies the adhesive strength of the substrate. The adhesion gradients in the substrate, along with hydrodynamic interactions among the capsules, gives rise to a sustained motion of the microcapsules. In this work, we perform simulations (based on lattice Boltzmann method for the fluid and random walk simulation for nanoparticles) of several signal-target configurations, consisting of two or more rigid capsules. In particular, we examine a configuration consisting of a single signaling capsule pushing multiple target capsules in a single file. For a constant release rate of nanoparticles, the velocity of the train of capsules asymptotes to a constant value at large times. Using a low-order analytical model for this system, we find that there is a simple relationship between this asymptotic velocity and the parameters in the system (e.g. number of capsules, release rate of nanoparticles, viscosity of fluid, adhesive strength of substrate etc.).

9:12AM P15.00007 Mixing fluid by self-propelled objects, MAXIM BELKIN, Illinois Institute of Technology / Argonne National Lab, ALEXEY SNEZHKO, IGOR ARANSON, WAI-KWONG KWOK, Argonne National Lab — Magnetic microparticles suspended at the water-air interface and subjected to an ac external driving self-assemble into dynamic structures (magnetic snakes). The snakes are accompanied by four large hydrodynamic vortices. At high enough frequencies and amplitudes of driving the snakes transform into self-propelled swimmers. Moving erratically, these swimmers mix the surface of fluid at a very high rate. We performed detailed experimental studies of these self-organized mixing. We studied space and time correlation and diffusion process in such systems.

9:24AM P15.00008 Enskog-theory for stochastic models with self-propelled and passive particles, ALEMAYEHU GEBREMIHARI, THOMAS IHLE, Department of Physics, North Dakota State University — Macroscopic evolution equations for interacting many-body systems do not just “emerge”; they follow from microscopic laws. However, it is often difficult to quantitatively establish this link, especially for systems which cannot be described by a Hamiltonian and which do not have pairwise additive interactions. Therefore, the general form of the macroscopic equations is usually obtained by symmetry arguments. Here, using a particle-based model with discrete time evolution steps for fluid flow I show how the macroscopic transport equations can be rigorously derived from microscopic collision rules. The approach starts with the full N-particle Liouville equation and leads to a multi-particle Enskog-equation which is treated by a Chapman-Enskog expansion. No linearization or single-relaxation time approximation of the collision operator are needed. The obtained thermo-hydrodynamic equations show excellent agreement with previous numerical results. The same approach is used to study a simple model of self-propelled, swimming birds. This model was proposed by T. Vicsek et al. [Phys. Rev. Lett. 75 (1995) 1226]; it has “multi-particle collisions” where birds within some interaction range align their flying directions. I analytically analyze the collision-operator for small and large bird density, and derive the hydrodynamic equations for the density and velocity fields.

Footnotes:
†This work was supported by the US DOE, grant DE-AC02-06CH11357.
9:36AM P15.00009 The “caterpillar” simulation model for a biological filament1, AIMIE BAILEY, Imperial College London, CHRISTOPHER LOWE, Universiteit van Amsterdam, ADRIAN SUTTON, Imperial College London — We present a simulation model for an elastic filament in a viscous fluid, relevant for systems ranging from suspensions of paper pulp to micro-organism motility. It incorporates the Stokeslet treatment of the hydrodynamic force. We show that a non-arbitrary choice of the hydrodynamic radius is necessary to recover known dynamic behavior of a fiber with a finite cross-section. Our simulations explore configurations inaccessible by theory. We illustrate the utility of the model by considering the simple scenario of a charged filament in an electric field. Results suggest a circularly polarized electric field is a viable means for aligning microtubules in solution.

1 A.G.B. thanks the Thouron Award and the NSF Graduate Research Fellowship Program for support.

9:48AM P15.00010 Flow and nutrient transport through porous scaffolds used for the culture of bone cells in perfusion bioreactors1, 2, 3, DIMITRIOS PAPAVASSILIOU, The University of Oklahoma, ROMAN VORONO, VASSILIOS SIKAVITAS, The University of Oklahoma, SAMUEL VANGORDON — The goal is to understand via computation the behavior of the flow inside porous scaffolds that are used for bone tissue engineering. Fluid shear is an important stimulatory factor in preosteoblastic cells seeded in scaffolds and cultured under flow perfusion. A Lattice Boltzmann method has been employed to simulate the flow field within porous scaffolds obtained with high resolution micro-CT. Lagrangian methods have also been used to determine the nutrient dispersion inside the scaffolds. The shear stresses calculated inside the scaffold architecture indicate that the shear stresses experienced by cells inside the scaffold can vary by orders of magnitude. This is important when designing scaffolds for bone tissue engineering as it could effect the behavior of the scaffold. Moreover, cell detachment can occur when the fluid shear is too high, thus placing a limit on the stresses that a particular scaffold design should allow. The talk will address the methodology, the validation and the correlation of scaffold structure characteristics with the shear stresses and with the rate of mass transfer.

1 NSF (CBET-0700813) and TeraGrid support (TS080042)

10:00AM P15.00011 Instabilities and waves in thin films of living fluids, SUMITHRA SANKARARAMAN, SRIRAM RAMASWAMY — We formulate the thin-film hydrodynamics of a suspension of polar self-driven particles and show that it is prone to several instabilities through the interplay of activity, polarity and the existence of a free surface. Our approach extends, to self-propelling systems, the work of Ben Amar and Combettes [Phys Fluids 13 (2001) 1160] on thin-film nematics. Based on our estimates the instabilities should be seen in bacterial suspensions and the lamellipodium, and are potentially relevant to the morphology of biofilms. We suggest several experimental tests of our theory.

10:12AM P15.00012 Tuning inter-virus interactions in natural aquatic environments, NATHAN W. SCHMIDT, Department of Physics, University of Illinois, Urbana-Champaign, ANDREW K. UDIT, Department of Chemistry, Scripps Research Institute, LEONARDO GUTIERREZ, THANH H. (HELEN) NGUYEN, Civil and Bioengineering, University of Illinois, Urbana-Champaign, M.G. FINN, Department of Chemistry, Scripps Research Institute, GERARD C.L. VONG, Department of Materials Science and Engineering, University of Illinois, Urbana-Champaign — Polymeric natural organic matter (NOM) originating from plants and animals is ubiquitous in natural aquatic environments. Many water-borne pathogens, including viruses, readily associate with NOM, which has a statistic distribution of charged and hydrophobic groups. Virus-NOM association influences the transport of viruses in groundwater environments, but little is known about this interaction, or how NOM can induce new inter-virus interactions. To better understand the interaction between NOM and aqueous contaminants, we use the MS2 and Qbeta viruses (diameters ~ 27nm) as surrogate water-borne pathogens. Smal Angle X-Ray Scattering is used to characterize the inter-particle interaction between viruses over a range of NOM concentrations and different salt types and concentrations.

10:24AM P15.00013 Computational studies on characteristic fluid behavior in the stented cerebral aneurysm, MIKI HIRABAYASHI1, University of Geneva, MAKOTO OHTA2, DANIEL A. RÜFENACHT3, Hospital University of Geneva, BASTIEN CHOPARD, University of Geneva — We present a computational analysis of the fluid behavior in the stented aneurysm. It is important to reveal the complex mechanism of the velocity reduction of the flow in the stented aneurysm in order to design the effective stent, which is a tubular mesh of wires placed for the treatment of the cerebral aneurysm. To understand the effect of a stent we already proposed a qualitative analysis of the flow pattern in the stented aneurysm. Here we present a quantitative analysis of the transition of the pressure and the shear stress caused by the changes of the flow pattern to verify the velocity reduction mechanism of the stent. We expect that our study will lead to a new suggestion for the effective treatment of the cerebral aneurysm by the stent.

1 NICT (present affiliation)
2 University of Tohoku (present affiliation)
3 Hirslanden Clinic (present affiliation)

10:36AM P15.00014 Run length is the dimension that characterizes path integrals useful for designing passive bacterial pumps1, DAVID LIAO, GUILLAUME LAMBERT, Department of Physics, Princeton University, Princeton, NJ 08544, PETER GILADAJA, Delft University of Technology, C.J. Delft, The Netherlands, ROBERT AUSTIN, Department of Physics, Princeton University, Princeton, NJ 08544 — Asymmetric funnels have been used as passive pumps to concentrate E. coli in nanofabricated devices (Austin 2007). Funnel geometry changes pump efficiency, which could be important when driving cell sorters (Whitesides 2008). The large set of funnel geometries that could be considered when designing pumps motivated us to derive a path-integral-like formula to predict the flux produced by arbitrary funnel geometries. We applied this equation to a two-dimensional wedge-shaped funnel. Model and experiment agree that the steady-state ratio between concentrations on two sides of a funnel open to 60° is 3 when the aperture is one fifth the bacterial run length and 1 when the aperture is 16 times the run length, an example of how the run length here has a role loosely analogous to the wavelength in quantum mechanical path integrals.

1 Partial support by and performance at the CNF ECS-0335765, NBTC ECS-9876771, DARPA, NSERC, and NDSEG

10:48AM P15.00015 Selective transport through nano-channels: do we understand it?, ANTON ZILMAN, Los Alamos National Laboratory, T. JOVANOVIC-TALISMAN, B. CHAIT, M. ROUT, S. DI TALIA, M. MAGNASCO, Rockefeller University — Functioning of living cells requires selective molecular transport, which is provided by transport channels that are able to selectively transport certain molecular species while filtering others, even similar ones. Such channels can selectively transport their specific molecules in the presence of vast amounts of non-specific competition. In many cases, efficient and selective transport occurs without direct input of metabolic energy and without transitions from an ‘open’ to a ‘closed’ state during the transport event. Examples include selective permeability of porins and transport through the nuclear pore complex. Mechanisms of selectivity of such channels have inspired design of artificial selective nano-channels, which mimic the function of selective biological channels. Mechanisms of selectivity of such nano-channels are still unknown. I present a theoretical model to explain the selectivity of transport through nano-channels, which contains only the essentials of stochastic kinetics inside the channel. The theory provides a mechanism for selectivity based on the differences in the kinetics of transport through the channel between different molecules. The theory explains how the specific molecules are able to filter out the non-specific competitors - and proposes a mechanism for sharp molecular discrimination. The theoretical predictions account for previous experimental results and have been verified in ongoing experiments.
Wednesday, March 18, 2009 8:00AM - 10:00AM –
Session P16 DAMOP: Solid Helium: Theory 317

8:00AM P16.00001 Simulating the Melting Transition of Helium in Two Dimensions , KEOLA WIERSCHEN, MARTECH & Department of Physics, Florida State University, EFSTRATIOS MANOUSAKIS, MARTECH & Department of Physics, Florida State University and Department of Physics, University of Athens, Greece — We study the melting behavior of helium in two dimensions with the path integral Monte Carlo method. Two dimensional melting theory predicts two melting transitions: solid to hexatic and hexatic to isotropic liquid, described by a loss of translational and orientational order, respectively. We calculate the translational and orientational order parameters, and use finite size scaling to determine the two melting transitions in the thermodynamic limit. We also study the superfluid/normal phase boundary of 2D helium relative to the above mentioned two stage melting boundaries.

8:12AM P16.00002 Superfluid networks with mesoscopic structure as models of supersolid 4He , BURCU YUCESOY, JON MACHTA, NIKOLAI PROKOF’EV, BORIS SVISTUNOV, U. Massachusetts Amherst — One proposal for understanding supersolidity is that grain boundaries and/or defect lines in solid 4He may support superfluidity. To understand the consequences of this proposal, we carry out simulations of the XY model with mesoscale structure corresponding to grain boundaries and/or defect lines. In the absence of disorder, we find a sharp phase transition unlike the gradual transition seen in experiments on supersolids. However, with disorder we find results that are qualitatively similar to the experiments.

8:24AM P16.00003 Absence of Dislocation Quantum Roughening in Solid 4He , DARYA ALENIKAVA, EUGENE DZEDZITS, ANATOLY KUKLOV, CSI, CUNY, DAVID SCHMELTZER, CCNY, CUNY — Dislocations in quantum crystals are shown to be smooth at zero temperature because of the effective Coulomb-type interaction between kinks induced by exchange of bulk phonons. We provide heuristic Kosterlitz-Thouless and Renormalization Group arguments against quantum roughening and confirm them by Monte Carlo simulations of the effective model of edge dislocation moving in its gliding plane - a quantum string (or classical membrane in d = 2) subjected to periodic Peierls potential and Coulomb-type interaction. Simulations of such Sine-Gordon type action have been conducted in the Villain approximation in terms of the J-current formulation. Renormalized stiffness as a function of the long-range interaction strength C and dislocation length L is shown to be described by a master curve $F(C/L, x)$, where $F(x) \to 0$, as $x \to \infty$. We also discuss a mechanism of suppression of superfluidity along the dislocation core by thermal kinks and show that it leads to locking in of the mechanical and superfluid responses at finite temperature, which is consistent with the recent experiment of Day and Beamish (Nature 450, 853 (2007)).

8:36AM P16.00004 Classical roughening of dislocations and the effect of shear modulus softening in solid 4He , EUGENE DZEDZITS, DARYA ALENIKAVA, ANATOLY KUKLOV, CSI, CUNY, DAVID SCHMELTZER, CCNY, CUNY — We propose that shear modulus $\mu(T)$ softening with increasing temperature $T$ observed by Day and Beamish [1] is due to a crossover experienced by dislocations from quantum smooth to classically rough state in the Peierls potential. Quantum dislocation is described by the Sine-Gordon model in dimensions $d = 1 + 1$ with long-range interactions between kinks (induced by exchanging bulk phonons). Monte Carlo simulations of this model show that finite $T$ response on external stress can fit well the data $\mu(T)$ [1] for the parameters typical for 4He. We compare this model with the one proposed in Ref. [1]: the 4He impurities boiling off from the dislocations. Good fit of $\mu(T)$ cannot be achieved within this model for realistic values of the dislocation densities and relative fractions of 4He atoms. [1] J. Day and J. Beamish, Nature 450, 853(2007)

1 We acknowledge support from NSF grant PHY 0653135 and CUNY grant 80209-0914.

8:48AM P16.00005 Quantum Glass in Solid He71 , ALEXANDER BALATSKY, MATTHIAS GRAF, LANL — Recent discovery of a possible supersolid state by Kim and Chan has stimulated an active debate about true nature of a low temperature state of solid 4He. We will discuss possible glassy component that could be present in solid 4He. We will focus on i) the role of tunneling systems (TS) as a component that freezes out at lowest temperatures and ii) interactions between TS. We will address possible quantum effects and the role of TS statistics in solid 4He vs solid 3He-4He mixtures. Implications for the torsional oscillator and for thermodynamics will be discussed as well.

2 Work Supported by US DOE

9:00AM P16.00006 The glassy response of torsion oscillators of solid 4He , MATTHIAS J. GRAF, LANL, ZOHAR NUSSINOV, WUSTL, ALEXANDER V. BALATSKY, LANL — We have calculated the glassy response of a torsional oscillator filled with solid 4He assuming a phenomenological glass model. Making only a few assumptions about the distribution of glassy relaxation times in a small subsystem of otherwise rigid solid 4He, we can account for the bulk of the magnitude of the observed period shift and dissipation peak as reported in several torsion oscillator experiments. The glass model places stringent constraints on dynamic and thermodynamic responses of solid 4He and the magnitude of a possible supersolid phase. We also discuss the implications for a superglass state proposed recently by the Cornell group.

3 Supported by parts by LDRD of LANL and CMI of WUSTL.

9:12AM P16.00007 A ‘Superglass’ State in Solid 4He , BENJAMIN HUNT, ETHAN PRATT, VIKRAM GADAGKAR, Cornell University, MINORU YAMASHITA, Kyoto University, ALEXANDER V. BALATSKY, T-Division, Center for Integrated Nanotechnologies, Los Alamos National Lab, J. C. DAVIS, Cornell University, Brookhaven National Laboratory, University of St Andrews — We study the relaxation dynamics of both the resonance frequency $f(T)$ and the dissipation rate $D(T) = Q^{-1}(T)$ of a torsional oscillator (TO) containing solid 4He. Abruptly at the temperature $T^*$ characteristic of the proposed supersolid phase, the relaxation times within $f(T)$ and $D(T)$ begin to increase precipitously together. Moreover, for all $T < T^*$, relaxation processes in both $D(T)$ and a component of $f(T)$ exhibit a synchronized ultra-slow evolution towards equilibrium and strong thermal hysteresis. We demonstrate that, while reminiscent of glassy dynamics, these phenomena are quantitatively inconsistent with a simple freeze-out transition because the variation in $f$ is far too large. We conclude that, if solid 4He exhibits a superfluid component, this system represents a new form of quantum matter – a complex supersolid in which a crystalline excitation exhibiting glassy dynamics controls the superfluid phase stiffness.

3 These studies are supported by National Science Foundation under Grant DMR 434801; B.H. acknowledges support by NSERC; M.Y. acknowledges support from the JSPS.
We model the torsional oscillator experiments by using the Kelvin-Voigt model of viscoelasticity for solid $^3$He [1]. Recent heat capacity experiments on solid $^4$He [2] show a peak in the specific heat which is interpreted as the signature of the supersolid transition. We pursue an alternative explanation for the heat capacity feature in which $^3$He impurities desorb from dislocations in solid $^4$He; the peak temperature scales with the binding energy of $^3$He to dislocations in $^4$He. Within a continuum elastic model for solid $^4$He, we make quantum mechanical estimates for the binding energy, using a combination of variational and numerical methods. We find for a short distance cut-off of one lattice constant of $^4$He, the binding energy is about 70 mK for edge and 60 mK for a screw dislocation. [1] X. Lin, A. C. Clark, and M. H. W. Chan, Nature 449, 1025 (2007).

This work is supported by the NSF.

Specific heat due to the binding of $^3$He impurities to dislocations in solid $^4$He.

This work is supported by the NSF.

Specific heat due to the binding of $^3$He impurities to dislocations in solid $^4$He.

This work is supported by the NSF.

Practical elimination of leakage in superconducting qubits by pulse shaping.

This work is supported by MITRE Technology Program.

Quantum Sensing in the Presence of Realistic Attenuation.

The authors wish to thank CREST, JST for funding.
8:36AM P17.00004 Quantum multiobservable control . RAJ CHAKRABARTI, Princeton University, REBINDING WU, Tsinghua University, HERSHEYEL RABITZ, Princeton University — We present deterministic algorithms for the simultaneous control of an arbitrary number of quantum observables. Unlike optimal control approaches based on cost function optimization, quantum multiobservable tracking control (MOTC) is capable of tracking predetermined homotopic trajectories to target expectation values in the space of multiobservables. The convergence of these algorithms is facilitated by the favorable critical topology of quantum control landscapes. Fundamental properties of quantum multiobservable control landscapes that underlie the efficiency of MOTC, including the multiobservable controllability Gramian, are introduced. The effects of multiple control objectives on the structure and complexity of optimal fields are examined. With minor modifications, the techniques described herein can be applied to general quantum multiobjective control problems.

8:48AM P17.00005 Quantum speed limit and optimal control . TOMMASO CANEVA, International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste, Italy, MICHAEL MURPHY, TOMMASO CALARCO, Institut für Quanteninformationsverarbeitung, Universität Ulm, D-89069 Ulm, Germany, ROSARIO FAZIO, NEST-CNR-INFN & Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy, SIMONE MONTANGER, Institut für Quanteninformationsverarbeitung, Universität Ulm, D-89069 Ulm, Germany, VITTORIO GIOVANETTI, NEST-CNR-INFN & Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy, GIUSEPPE E. SANTORO, International School for Advanced Studies (SISSA), Via Beirut 2-4, I-34014 Trieste, Italy — The Heisenberg uncertainty principle, $\Delta E \Delta t \geq \hbar$, implies that a system cannot pass through distinguishable, i.e. orthogonal, states within arbitrarily short time. In the case of a time-independent Hamiltonian, the presence of this ultimate bound has been well established and summarized in the concept of a maximum allowed velocity, called quantum speed limit (QSL). On other hand for a time-dependent Hamiltonian the problem started to be addressed only very recently and is still open. Optimal control theory offers a valuable tool to explore this issue: we test its performance in two paradigmatic cases, Landau-Zener model and transfer of information along a chain of coupled spins, and show that the results are compatible with the ultimate limits enabled by quantum mechanics.

9:00AM P17.00006 Performance Gains for Superconducting Qubits by Means of Optimal Control Theory1. ROBERT ROLOFF, WALTER POETZ, Karl-Franzens-Universitaet Graz — Superconducting circuits are promising candidates for the successful implementation of qubit-arrays and qubit-gates within solid-state systems. However, despite recent progress within coherent control of charge, phase and flux qubits, considerable improvement in gate fidelities is needed to build large-scale quantum information processing devices. We present an optimal control scheme based on process tomography, capable of taking into account relaxation, dephasing and unwanted state-leakage within the qubit (array). We apply this theory to explore the performance limits of Josephson charge qubits within current experimental means. Environmental effects, as well as state-leakage, are modeled microscopically, using a fully quantum mechanical description and taking into account $1/f$ and Ohmic fluctuations based on experimental noise spectra. Within time-optimal control theory, we show that under typical conditions gate fidelities of $F = 1 - 10^{-3}$ should be possible for a Josephson charge qubit. 1The authors wish to acknowledge financial support of this work by FWF Project P18829.

9:12AM P17.00007 Towards non-adiabatic quantum control of a superconducting qubit . JONAS BYLANDER2, MARK S. RUDNER1, ANDREY V. SHYTOV2, SERGIO O. VALENZUELA1, DAVID M. BURNS1, KARL K. BERGGREN1, LEONID S. LEVITOV1, WILLIAM D. OLIVER1. 1Massachusetts Institute of Technology, 2University of Utah — Transitions in a qubit driven through an energy-level avoided crossing can be controlled by carefully engineering the driving protocol. With the driving rate chosen to optimize the coupling strength, an arbitrary rotation of a qubit’s quantum state on the Bloch sphere can be performed. This regime, if realized experimentally, may lead to fast quantum-logic gates with times of operation much shorter than those achieved by using Rabi transition-based protocols. We have performed an experiment with a superconducting persistent-current qubit in the non-adiabatic regime, driven by a large-amplitude radio-frequency field. By applying a waveform consisting of two harmonic components generated by a digital source, we demonstrate a mapping between the amplitude and phase of the harmonics produced at the source and those received by the device. This mapping allows us to image the actual waveform at the device and accurately determine the desired time dependence. Our method constitutes a step towards non-adiabatic control with arbitrary waveforms.

9:24AM P17.00008 Universal quantum control of two electron spin qubits via dynamic nuclear polarization . HENDRIK BLOHM, SANDRA FOLETTI, Harvard University, DIANA MAHALU, VLADIMIR UMANSKY, Weizmann Institute of Science, AMIR YACOBY, Harvard University — Encoding a single logical qubit in the collective spin states of two electrons in a double quantum dot can provide sub-nanosecond electrically controlled gates that are fast enough to refocus dephasing due to slow fluctuations of the hyperfine field from the nuclei of the host material [1]. In this work, we experimentally demonstrate full quantum control of a GaAs two electron logical spin qubit. One fast electrical control axis resulting from coherently exchanging the two electrons has already been demonstrated [2]. We achieve coherent evolution around a second axis caused by a difference in the nuclear hyperfine fields felt by the two electrons. This field difference is obtained by dynamically polarizing the Ga and As nuclei by transferring spin from the electrons to the nuclei. It can reach up to several hundred mT and can be maintained in a steady state. We demonstrate rotations around this axis with a programmable frequency that can exceed 1 GHz. Using quantum state tomography enabled by both control axes, we characterize the evolution of the qubit state around a fixed but tunable combined axis. Our results establish full electrical quantum control at the single qubit level with gate times of a few nanoseconds. [1] Taylor et al., Nature Physics 1, 177 (2005). [2] Petta et al. Science 309, 2180 (2005).

9:36AM P17.00009 Control of exchange coupling in Si double quantum dots1. DAMITRIE CULCER, L. CYWINSKI, QIUZI LI, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park MD 20742 — We determine the exchange coupling in a Si double quantum dot in the Heitler-London approximation. Qubit manipulation in bulk Si is hindered by the sixfold valley degeneracy of conduction band electrons which causes the exchange interaction between qubits to oscillate as a function of their separation. We demonstrate that in quantum dots these oscillations are suppressed by quantum confinement. We determine the dependence of the exchange coupling on the barrier potential between the dots and examine the role of charge fluctuations. Our results suggest that together with long Si spin lifetimes Si quantum dots could lead to improved control of spin qubits. Within the Heitler-London approximation the work presented is completely general and the results are valid for any ground state. 1Work supported by LPS-NSA.
9:48AM P17.00010 Optimal experiment design for parameter estimation as applied to dipole- and exchange-coupled qubits\textsuperscript{1}, KEVIN YOUNG, MOHAN SAROVAR, BIRGITTA WHALEY, University of California - Berkeley, ROBERT KOSUT, SC Solutions — We consider the problem of quantum parameter estimation with the constraint that all measurements and initial states are separable. Two qubits are presumed coupled through the dipole and exchange interactions. The resulting Hamiltonian generates a unitary evolution which, when combined with arbitrary single-qubit operations, contributes to a universal set of quantum gates. However, while the functional form of the Hamiltonian is known, a particular experimental realization depends on several free parameters - in this case, the position vector relating the two qubits and the magnitude of the exchange interaction. We use the Cramer-Rao bound on the variance of a point estimator to construct the optimal series of experiments to estimate these free parameters. Our method of transforming the constrained optimal estimation problem into a convex optimization is powerful and widely applicable to other systems.

\textsuperscript{1}Supported by NSF Grant No. MOD713106A

10:00AM P17.00011 Measurement of the nonadiabatically-induced coherent time evolution of a single-electron wavefunction in a surface acoustic wave dynamic quantum dot , ADAM THORN, MASAYA KATAOKA, MICHAEL ASTLEY, University of Cambridge, UK, DANIEL OI, University of Strathclyde, UK, CRISPIN BARNES, CHRIS FORD, DAVE ANDERSON, GEB JONES, IAN FARRER, DAVE RITCHIE, MICHAEL PEPPER, University of Cambridge, UK — Observation of coherent single-electron dynamics is severely limited by experimental bandwidth. We present a method to overcome this using moving quantum dots defined by surface acoustic waves. Each dot holds a single electron, and travels through a static potential landscape. When the dot moves abruptly between regions of different confinement, the electron is excited into a superposition of states, and oscillates unitarily from side to side. These oscillations are measured almost non-invasively, by allowing a small amount of tunnelling out of the dot each time the wavefunction approaches a tunnel barrier. We have modelled this in detail by solving the single-particle time-dependent Schrödinger equation for a realistic potential, and find good agreement between the measurements and the simulations.

10:12AM P17.00012 Weak measurement of a solid-state qubit revealed in low-frequency noise\textsuperscript{2}, ALEXANDER KOROTKOV, University of California, Riverside — Weak quantum measurement becomes a subject of experimental study with solid-state qubits. Partial collapse, quantum uncollapsing, and persistent Rabi oscillations have been already demonstrated with superconducting qubits by the UCSB and Saclay groups. Now we propose an experiment, in which the features of a weak quantum measurement are revealed in the low-frequency noise of the detector signal. (Here we mean a frequency much lower than the Rabi frequency, though sufficiently high to avoid 1/f noise.) The idea is to use two detectors measuring the same qubit, so that one detector collapses the qubit, while the other detector senses the result of the collapse. Then the cross-correlation of low-frequency noises in outputs of the two detectors carries information about the collapse process. The experiment can be realized with superconducting or semiconductor qubits.

\textsuperscript{2}Supported by NSA/IARPA/ARO grant

10:24AM P17.00013 Error Accounting in Electron Counting Experiments\textsuperscript{1}, MICHAEL WULF, ALEXANDER B. ZORIN, Physikalisch Technische Bundesanstalt — Electron counting experiments attempt to provide a current of a known number of electrons per unit time. We propose architectures utilizing a few readily available electron-pumps or turnstiles with error rates of 1 part in 10\textsuperscript{8} with common sensitive electrometers to achieve the desirable accuracy of 1 part in 10\textsuperscript{4}. This is achieved not by counting electrons but by counting the errors of individual devices; these are less frequent and therefore readily recognized and then accounted for. We thereby ease the route towards quantum based standards of current and capacitance.

\textsuperscript{1}Supported in part by the EU under projects EuroSQIP and REUNIAM.

10:36AM P17.00014 High-fidelity universal quantum gates through quantum interference , FRANK GAITAN, Southern Illinois University, RAN LI — Numerical simulation results are presented which suggest that a class of non-adiabatic rapid passage sweeps first realized experimentally in 1991, and which give rise to controllable quantum interference effects observed in 2003 using NMR, should be capable of implementing a universal set of quantum gates $g$ that operate with high-fidelity. $g$ consists of the Hadamard and NOT gates, together with variants of the phase, $\pi/8$, and controlled-phase gates. Sweep parameter values are provided which simulations indicate will produce the different gates in $g$, and for each gate, yield an error probability $P_e < 10^{-4}$. These simulations suggest that the universal gate set produced by these rapid passage sweeps show promise as possible elements of a fault-tolerant scheme for quantum computing. We discuss current challenges facing experimental implementation of this approach to universal quantum computing.

10:48AM P17.00015 Dynamics of Quantum Control for Bosons in Optical Lattices\textsuperscript{1}, ANALABHA ROY, Graduate Student, University of Texas at Austin, LINDA REICHL, Director, CQS University of Texas at Austin — We investigate the possibility of quantum control in an ultracold atom Bose gas in an optical lattice by looking at numerical simulations of the dynamics of controlled excitations in these systems. These excitations are mediated by pulsed signals that cause Stimulated Raman Adiabatic passage (STIRAP) from the ground state to excited states. The transition to chaos affects the quantum dynamics of such systems as has been demonstrated for single-particle and mesoscopic-systems in optical potentials. We determine the influence of Bose statistics on this dynamics, as well as the effects of controlling quantum phase transitions in this manner for interacting cold atom systems.

\textsuperscript{1}The authors thank the Texas Advanced Computing Center (T.A.C.C.) at the University of Texas at Austin for the use of their high-performance distributed computing grid.

Wednesday, March 18, 2009 8:00AM - 11:00AM – Session P18 DPOLY: Bulk Block Copolymers II 319

8:00AM P18.00001 Directed Self-Assembly of Cadmium Selenide Nanocrystals in Conjugated Rod-Coil Block Copolymers , B. L. MCCULLOCH, Dept of Chemical Engineering, University of California-Berkeley, J. URBAN, Molecular Foundry, Lawrence Berkeley National Laboratory, R. A. SEGALMAN, Dept of Chemical Engineering, University of California-Berkeley — Semiconducting polymer/nanocrystal composites are attractive for many applications; however their performance relies crucially on nanoscale morphology. We demonstrate that a conjugated rod-coil diblock copolymer can be used both to absorb light and template the location of CdSe nanocrystals. A combination of the liquid crystallinity of the conjugated rod block and the interactions of the nanocrystal ligand coat with the block copolymer control self-assembly. For example, incorporation of the nanocrystal in the rod nanodomain disrupts liquid crystallinity. In the case of a poly(alkoxy-phenylene vinylene-b-2-vinyl pyridine) (PPV-b- P2VP) block copolymer and CdSe nanocrystals, self-assembly leads to a bulk lamellar structure on the 10nm length scale. Small angle X-ray scattering confirms the addition of nanocrystals swells the domain size. We demonstrate via transmission electron microscopy the nanocrystals reside preferentially in the P2VP domain, presumably due to the strong nanocrystal surface interactions with polar P2VP and exclusion effects of the crystalline PPV phase.
8:24AM P18.00003 Nano-porous Poly(3-hexylthiophene) films: A novel route to prepare bulk heterojunction photovoltaic devices, TIRTHA CHATTERJEE, KULANDAIVELU SIVANANDAN, CRAIG J. HAWKER, EDWARD J. KRAMER, Mitsubishi Chemicals-Center for Advanced Materials, Materials Research Laboratory, University of California, Santa Barbara, CA 93106 — Conjugated polymers are excellent candidates for use in low-cost electronics and photovoltaic applications. Bulk heterojunction (BHJ) morphologies are promising device architecture as the close proximity of the electron donor and acceptor micro-domains (with domain size comparable with the exciton diffusion length) facilitates the charge transport process. In order to achieve a well ordered BHJ architecture, poly(3-hexylthiophene) (P3HT) based rod-coil copolymers are synthesized where coil blocks are grafted to the P3HT chain through a cleavable linker. The linker and the attached sacrificial coil block can easily be cleaved and removed by chemical treatment leaving a rough nano-porous P3HT film. Scanning force microscopy and grazing incidence small angle X-ray scattering convincingly show the nano-pore formation. Further, depth profiling using dynamic secondary ion mass spectroscopy indicates that nano-pores probably penetrate the entire depth of the film (device thickness). Subsequently refilling of the nano-pores by electron transporting component (fullerene derivatives) provides the required device morphology.

8:36AM P18.00004 The Influence of Electric Fields on the Order-Disorder Transition Temperature of Block Copolymer Systems, HEIKO SCHOBERTH, Lehrstuhl fuer Physischale Chemie II, Universitaet Bayreuth, D-95440 Bayreuth, Germany, KRISTIN SCHMIDT, Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA, KERSTIN SCHMIDLER, ALEXANDER BÖKER, Lehrstuhl fuer Physischale Chemie II, Universitaet Bayreuth, D-95440 Bayreuth, Germany — We investigate the influence of electric fields on the phase behavior of diblock copolymers in concentrated solutions using synchrotron small-angle X-ray scattering (synchrotron SAXS). When heating the solutions through the order-disorder transition temperature $T_{ODT}$, we find a significant decrease in $T_{ODT}$ with increasing electric-field strength. In addition we found a temperature regime in which it is possible to switch between the mixed and phase separated state at constant temperature upon application of a moderate electric field.

3This work was carried out in the framework of the SFB 481 (TP A2) funded by the German Science Foundation (DFG). AB acknowledges financial support by the Lichtenberg-Program of the VolkswagenStiftung.

8:48AM P18.00005 Phase Behavior of Polystyrene-block-Poly(n-alkyl-ran-n’alkyl methacrylate) Copolymers, HONG CHUL MOON, JUNHAN CHO, Dankook University, JIN KON KIM, Pohang University of Science and Technology — The phase behavior of polystyrene-block-poly(n-butyl-ran-n’-hexyl) methacrylate copolymers and polystyrene-block-poly(n’-octyl-ran-methyl) methacrylate copolymers were investigated by using small angle X-ray scattering, birefringence and rheometry. When the total molecular weight and the composition of the random copolymers were judiciously controlled, the closed-loop phase behavior with both a lower disorder-to-order transition and an upper order-to-disorder transition was observed. These block copolymers exhibited excellent baroplasticity. The observed phase behavior was explained by a compressible mean field approach.

3This work was supported by Creative Research Initiative Program supported by KOSEF.

9:00AM P18.00006 Gas Pressure Effect on Phase Behavior of Deuterated Polystyrene-block-poly(n-pentyl methacrylate) Copolymers, HYE JEONG KIM, JIN KON KIM, Pohang University of Science and Technology, DU YEOL RYU, Yonsei University — The pressure effect of various gases on the phase transitions of deuterated polystyrene-block-poly(n-pentyl methacrylate) copolymer was investigated by small angle neutron scattering (SANS) and birefringence. With increasing helium gas pressure, the size of closed-loop consisting of both the lower disordered-to-ordered transition and the upper ordered-to-disordered transition was decreased, which is similar to the hydrostatic pressure effect. On the other hand, when nitrogen gas was used, the size of the closed-loop became larger with increasing pressure. These interesting results are explained by the binding energy calculation.

3This work was supported by Creative Research Initiative Program supported by KOSEF.

9:12AM P18.00007 Pressure Jump Studies of Block Copolymer Phase Transition in Selective Solvent, YONGSHENG LIU, RAMA BANSIL, Boston University, MILOS STEINHART, Institute of Macromolecular Chemistry, CZ Republic — Synchrotron based time-resolved small angle x-ray scattering (SAXS) was used to study the kinetics of the order-disorder transition (ODT) in a 39% (w/v) solution of a diblock copolymer of poly(styrene – isoprene) (SI 18-12) in diethylphthalate (DEP), a selective solvent for the PS block using pressure jump methods. The results show that the ODT temperature increases at about 20°/kbar with pressure. Time resolved pressure jump SAXS experiments were done to study the kinetics of disorder to BCC phase transition and the reverse transition. Pressure jump from 100 bar to 800 bar at 108 C from disordered state displayed a BCC structure at 30 seconds. Results of experiments with solvent viscosity increased by adding low molecular weight polystyrene will also be presented.

3Supported by NSF DMR. RB acknowledges IR/D support of NSF.

9:24AM P18.00008 Self-assembled Oniontype Multiferroic Nanostructures, SHENQIANG REN, ROBERT M. BRIBER, MANFRED WUTTIG, Dept. of Mater. Sci. & Engi. University of Maryland, College Park — Spontaneously self-assembled oniontype multiferroic nanostructures based on block copolymers as templating materials are reported. Diblock copolymer containing two different magnetoelectric precursors separately segregated to the two microdomains have been shown to form well-ordered templated lamellar structures. Onion-type multilamellar ordered multiferroic (PZT/CeFe$_2$O$_4$) nanostructures have been induced by room temperature solvent annealing in a magnetic field oriented perpendicular to the plane of the film. The evolution of the onion-like microstructure has been characterized by AFM, MFM, and TEM. The structure retains lamellar periodicity observed at zero field. The onion structure is superparamagnetic above and antiferromagnetic below the blocking temperature. This templating process opens a route for the development of materials that will contribute to novel future technologies. Polymers can act as hosts for metallic and dielectric nanoparticles as well as organic molecules, resulting in nanocomposites with combinations of properties not available by other means. Periodic structural assemblies are of particular interest, due to their interesting interactions with waves: especially light and mechanical waves. Progress in this exciting area requires excellent control of structure formation. A top-down, bottom-up approach, using interference lithography and self assembly is demonstrating good success in fabricating the requisite structures and desired properties for photonics and phononics.

9:36AM P18.00009 Periodic Polymers for PhoXonics, EDWIN THOMAS, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Exploiting the size and shape dependence of material properties and accessing multi-functionality holds great promise for the development of materials that will contribute to novel future technologies. Polymers can act as hosts for metallic and dielectric nanoparticles as well as organic molecules, resulting in nanocomposites with combinations of properties not available by other means. Periodic structural assemblies of particular interest, due to their interesting interactions with waves: especially light and mechanical waves. Progress in this exciting area requires excellent control of structure formation. A top-down, bottom-up approach, using interference lithography and self assembly is demonstrating good success in fabricating the requisite structures and desired properties for photonics and phononics.
9:48AM P18.00010 Hydration and phase separation of polyethylene glycol in copolymers of tyrosine derived carbonates, N. SANJEEVA MURTHY, Rutgers University, WENJIE WANG, University of Vermont, JOACHIM KOHN, Rutgers University — Effect of PEG fraction and its block size on the temperature-induced phase transitions and the hydration-induced phase separation were investigated in a copolymer of desaminotyrosyl tyrosine ethyl ester (DTE) and PEG using simultaneous SAXS/WAXS/DSC. The PEG segments crystallized when the block size was at least 2000 Daltons and present at ~ 40 wt%, and raised the Tg of the polymer by ~ 15 °C. The PEG blocks in dry polymers with up to 50 wt% PEG, even when crystalline, were found to be uniformly distributed without evidence of phase separation at 10 nm length scales. The non-iodinated PEG-rich sample with 30 mole% PEG20k showed the lower critical solution temperature (LCST) behavior with PEG blocks forming a separate phase above ~21 °C. In the iodinated version of this polymer, the PEG20k blocks were phase separated in the solid phase. In all samples, whether PEG was crystalline or not, hydration induced PEG to separate into 15 nm hydrated domains. Phase behavior was dependent on whether poly(DTE) or the PEG was the major (matrix) phase. Changes in the mobility of the chains brought about by water-mediated hydrogen-bonding, and modulated by heat, appear to be the common underlying explanation for the range of observed phase behavior.

10:00AM P18.00011 Robustness of Pluronic Block Copolymer Nanostructure to Structural Changes in Dispersed Nanoparticles, THERESA A. LAFOLLETTE, LYNN M. WALKER, Carnegie Mellon University — Thermoreversible block copolymers [(PEO)n-(PPO)m-(PEO)n; trade name Pluronic] self assemble into ordered micelle gels. Nanoparticles (3-10nm) are templated in the interstitial spaces of Pluronic micelle gels to form nanocomposite systems. Globular hydrophilic proteins have served as model monodisperse nanoparticles in this work. We have shown that these proteins are templated in the interstitial sites of the cubic packed micelle gels at room temperature. By raising the temperature, the proteins are denatured to study the robustness of the micelle gel to structural changes due to the unfolded protein. Nanoscale structure is determined from small angle neutron scattering (SANS). It was expected that any change in the nanoparticle size would cause a change in the packing of the Pluronic micelle gel. However in SANS experiments, the FCC and BCC Pluronic templates show no nanoscale structural differences between a room temperature sample and a sample that has been heated to denature the protein and then cooled back to room temperature. There is a change in the template at longer length scales as evidenced by a low q upturn in the scattered intensity. The robustness of the micelle gel at different length scales will be discussed.

10:12AM P18.00012 Phase behavior of block copolymer nanocomposites, GEORGE PAPAKONSTANTOPOULOS, Arkema Inc., ANALYTICAL AND SYSTEMS, ARKEMA INC. TEAM — Incorporating nanoparticles in block copolymers can allow the creation of a material with modified properties. In addition, the control of the nanoparticle location in a nanometer scale, can lead to novel applications for these materials. Although, the phase behavior of block copolymers in the bulk is well established, the effects of nanoparticles on their phase behavior, especially under confinement, are not well understood. We carried out a systematic study to investigate the self-assembly of block copolymer-nanoparticle composites using a coarse grain model. These systems are studied in the bulk and under confinement. The dependence of the location and distribution of the nanoparticles within the block copolymer as a function of particle-polymer interaction, size and shape were examined.

10:24AM P18.00013 Effect of Chain Architecture on Nanoparticle Miscibility in Block Copolymer Nanocomposites, JESSICA LISKAT, HYUNG JU RYU, ILHEM F. HAKEM, Carnegie Mellon University, RANGOU SOFIA, POLITAKOS NIKOLAOS, MISICRONIS KONSTANTINOS, APOSTOLOS NGERPOULOS, University of Ioannina — This contribution will present a combined experimental and theoretical analysis of the effect of block copolymer chain architecture on the miscibility and morphology of enthalpically neutralized particle additives. The chain architecture is found to be a critical parameter in facilitating particle dispersion imposing both direct as well as indirect constraints on the particle distribution. Continuous block configurations (such as the bridged midblocks in triblock copolymers) are found to inhibit particle compatibilization. Interestingly, the particle miscibility is found to be strongly affected by the configuration of the block adjacent to particle-filled domains (indirect constraint). In particular, incompatibility is observed for high branching densities in the adjacent domains (such as miktoarm chain architectures). A mean-field model will be presented to rationalize this observation as a consequence of segmental crowding that counteracts changes in the layer dimensions induced by particle sequestration.

10:36AM P18.00014 Rheological and Mechanical Properties of Crosslinked Block Copolymer Nanofiber and Polystyrene Blends, SUNGWON MA, YONATHAN THIO, Georgia Institute of Technology — The mechanical and rheological properties of blends of crosslinked and uncrosslinked poly(styrene)-b-poly(isoprene) copolymer with commercially available polystyrene were studied. Cylindrical morphology of PS-b-PI copolymer was employed for generating nanofiber morphology. Cold vulcanization process using sulfur monochloride (S2Cl2) was used to preserve the morphology. Blends of uncrosslinked PS-b-PI copolymer with neat polystyrene were also prepared. Both blend samples were prepared by solvent casting method with the filler contents varying between 0.5 and 10 wt%. The mechanical and rheological properties were characterized and the microstructures of the fiber and the systems were imaged. The dynamic moduli (G' and G") of the crosslinked system increased with increasing the fiber content compared to the uncrosslinked system. The results were compared to the rheological model by fitting to Cross-Williamson. This blend study indicated critical volume concentration of nanofiber between 5 and 10 wt% of nanofiber content.

10:48AM P18.00015 Well Ordered Polymer Melts with Sub 5-Nanometer Domains upon Blending Surfactants with Selectively Associating Additives, VIKRAM DAGA, University of Massachusetts Amherst, VIJAY TIRUMALA, Polymers Division, NIST, JAMES WATKINS, University of Massachusetts Amherst — Applications employing block copolymers such as templating mesoporous inorganic structures and patterning would benefit from reduction in domain size formed in well-ordered block copolymer templates. The extent to which the domain size can be reduced is limited by the minimum required segregation strength, χN, where N denotes the size of block copolymer chains and the domain size. We have shown that disordered block copolymer surfactants with molar mass less than 15 kg/mol, can be made to undergo disorder-to-order transition by blending selectively associating homopolymers as well as small molecule additives with multi-point, non-ionic interactions. Blending with selectively associating additives result in an increase in segregation strength χN through an increase in apparent χ. The resulting domain sizes were found to be as low as 5 nm which is significantly lower than that seen for a typical block copolymer template.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P19 DPOLY: The Physics of Polymer Nanocomposites: Properties 320

8:00AM P19.00001 Tuning optical properties of gold nanorods in polymer films through thermal reshaping, RUSSELL COMPOSTO, ERIC MILLS, YU LIU, University of Pennsylvania — The thermal reshaping of gold nanorods (NRs) in a poly(methyl methacrylate) (PMMA) nanocomposite film is controlled by UV-vis and TEM. To ensure dispersion, the NRs are modified with PEG brushes, and then dispersed in PMMA. Thermal annealing of the PMMA:NR film results in a blue shift of the longitudinal plasmon resonance, caused by a decrease in the length of the NR. The rate of the blue shift increases as temperature increases from 100 °C to 200 °C, and the longitudinal absorption peak approaches a constant value that scales linearly with temperature. We demonstrate a potential application by fabricating a device with a gradient in optical properties.

1 NSF/DMR and MRSEC Programs
8:12AM P19.00002 Quenching Photoluminescence in Single-Walled Carbon Nanotube/Copolymer Composite Materials, ANDREW SCHOCH, Material Science and Engineering Dept. Northwestern University, L. CATHERINE BRINSON, Mechanical Engineering Dept. Northwestern University, KENNETH R. SHULL, Material Science and Engineering Dept. Northwestern University — Single-walled carbon nanotubes (SWNTs) stabilized by A-B diblock and A-B-A triblock copolymers are excellent model systems for studying the relationship between nanotube dispersion and mechanical response. The SWNTs cannot be dispersed in the alcoholic solvent used here without the addition of copolymer. However, the B blocks are in good solvent conditions for all temperatures and the A blocks solvent quality decreases with decreasing temperature. This solvate quality difference drives the formation of micelles with A block cores at low temperatures. As verified by AFM, the micelles form homogeneous micelles in solutions by incorporating the SWNTs. The dispersion has also been verified with near-IR photoluminescence spectroscopy (NIR-PLS) and the mechanical properties of these materials have been examined with rheological methods. The elastic contribution to the shear modulus increases while at high temperatures which we attribute to an increase in the number of NT-NT contacts. We have attempted to verify this observation by simulating the high temperature environment in the NIR-PLS measurements and looking for quenching.

8:24AM P19.00003 Temperature measurements of inverse micelles coated in gold nanoparticles using fluorescence, CHAD DALEY, JAMES A. FORREST, RYAN SPELLER, TOEWS WILLIAM, PATRICK MCVEIGH, Dept. of Physics and Astronomy, University of Waterloo, TODD EMRICK, Dept. of Polymer Sciene and Engineering, UMass Amherst — When nanoparticles are subject to laser radiation they have the ability to efficiently absorb energy from the beam and transform this energy into heat. Photothermal therapy uses this phenomenon to irreparably damage tissue surrounding nanoparticle conjugates. Despite the promise of this technique, there is no consensus on the damage mechanism or even the local heating. Here we present an experiment designed to measure local temperatures achieved in such processes. Ligand covered Gold nanoparticles are used to stabilize inverse micelles containing fluorescence dye in the water component. The fluorescence intensity being temperature dependent provides us with a means of measuring the temperature of the micelles as a function of time immediately following a laser pulse.

8:36AM P19.00004 Magnetic and Optical anisotropy thiol-capped Au NPs embedded into a polymer, JOSE DE LA VENTA, MIGUEL ANGEL GARCIA, VIRGINIA BOUZAS, Materials Physics Dept. University Complutense, ANDREA PUCCI, GIACOMO RUGGERI, Chemistry and Industrial Chemistry Departmen. University of Pisa — The anisotropy at the nanoscale is achieved when the shape of the objects is not spherical such as in the case of nanorods, nanotubes or nanowires. However, when they are embedded in a macroscopic matrix, the random distribution destroys the anisotropy. In this work we study the possibility of induce optical and magnetic anisotropy in a system consisting of spherical thiol capped Au NPs embedded in a polymeric matrix. The ferromagnetic-like behavior arises from the bond between the Au-S atoms and the optical response is also highly dependent on these bonds. So, modifications in the environment and in these bonds could alter the behavior of the whole system. When the NPs are embedded in a polymeric matrix, which is stretched even 40 times in one direction, SQUID and UV/Vis measurements show that a macroscopic anisotropy in spite of the spherical shape of the NPs. EXAFS measurements confirm that there are modifications in the Au-S bonds along the stretched direction that are responsible of the induced macroscopic anisotropy.

8:48AM P19.00005 Stability of the double gyroid phase to nanoparticle polydispersity in polymer tethered nanosphere systems, CAROLYN PHILLIPS, CHRISTOPHER IACOVELLA, SHARON GLOTZER, University of Michigan — Recent simulations have shown that aggregating nanospheres functionalized with polymer “tethers” can self-assemble to form the double gyroid phase also seen in block copolymer and surfactant systems. Within the gyroid domain, the nanoparticles pack in icosahedral motifs, stabilizing the gyroid phase in a small region of the phase diagram[1]. We study the impact of nanoparticle polydispersity on the properties of the double gyroid phase [2]. Here we show that a low amount of polydispersity lowers the energy of the phase. A large amount of polydispersity raises the potential energy of the system, disrupts the icosahedral packing, and eventually, destabilizes the gyroid. A study of binary gyroids indicates that the inclusion of a small population of either smaller or larger nanospheres encourages low-energy icosahedral clusters. Using a new measure for determining the volume of a component in a microphase-separated system based on the Voronoi-tessellation, we show that polydispersity compacts the gyroid domain and lowers the average coordination of the nanospheres. [1] Iacovella, et al., PRE, 2007 [2] Phillips, et al., “Stability of the double gyroid phase to nanoparticle polydispersity in polymer tethered nanosphere systems, preprint.

9:00AM P19.00006 Experimental and computational investigation of percolation in complex polymer nanocomposites, DERRICK STEVENS, LORI DOWNEN, NCSU Dept. of Physics, RUSSELL GORG, NCSU Dept. of Textile Engineering, LAURA CLARKE, NCSU Dept. of Physics — The continuing development of polymer nanocomposites has led to increasingly complex morphology, such as the mats of composite nanofibers formed from electrospinning. The formation of particle networks within the composite volume that leads to enhanced properties, such as electrical conductivity, may be influenced by this complex sample geometry. In this work, experimental and computational efforts are utilized to understand and predict the percolation threshold (critical volume fraction) for two cases: single ultra-high aspect ratio fibers (where fiber diameter can be similar to the particle dimensions) and these same fibers arranged in a random mat with up to 80% porosity. 2D and 3D Monte Carlo simulations, modeled on the actual parameters of our experimental system [1], are utilized and the results are compared with our experimental findings. In particular, confinement to fibers increases the percolation threshold; however the multi-fiber pathways available in mats partially reduce this constraint [2]. [1] S.S. Ojha, D.R. Stevens, K. Stano, T. Hoffman, L.I. Clarke, R.E. Gorga, Macromolecules 41, 2509 (2008). [2] D.R. Stevens, L.I. Downen, L.I. Clarke, Phys. Rev. B in press (2008).

9:12AM P19.00007 Influence on Thermal Diffusivity through a Transformation of Nanotube-like Clay Platelets in Polymer Blends, SEONGCHAN PACK, TAKASHI KASHIWAGI, TADANORI KOGA, JONATHAN SOKOLOV, MIRIAM RAFAILOVICH, Department of Materials Science and Engineering, Stony Brook University — We have previously demonstrated that large aspect ratio nanoparticles such as clays or nanotubes can form in-situ grafts which become universal compatibilizing agents for polymer blends. Here we show how the same mechanism could be applied to producing flame retardant materials in the polymer matrix. In particular, the large aspect nanoclays prevent thermally induced phase segregation and disperse the flame retardants, which greatly decrease flammability and increase efficiency of the flame retardants during combustion due to a formation of ribbons-like structures. These structures could produce a larger thermal differential gradient between the two polymer phases, which could change a heat specific of the system during combustion. Therefore, a small addition of the nanoclays affects the huge reduction on heat release rate and the mass loss rates. Furthermore, using a small angle X-ray scattering (SAXS), a transmission electron microscopy (TEM), and a scanning electron microscopy (SEM) shows that the clay platelets could be transformed into tubular-like rods during combustion, which would increase of the thermal diffusivity in the polymer blend.
of Pennsylvania — The study of rod percolation behavior has resurfaced in recent years, because it explains electrical conductivity in polymer nanocomposites containing carbon nanotubes and metal nanowires. Common processing techniques result in fillers with L/D < 50, so traditional models, which are only strictly correct in the limit of L/D ~ ∞, are ineffective at predicting percolation in these systems. We present a simulation that constructs percolated networks of finite-aspect ratio rods and calculates their electrical conductivity. We will compare our simulation results with polymer composites containing silver nanowires with aspect ratios of ~10 and ~30. Finally, we will present the temperature-dependent electrical conductivity of these composites and interpret the results using the thermal expansion coefficients of polyethylene and silver. These materials act as “thermal switches,” wherein electrical conductivity of certain composites can be manipulated by several orders of magnitude over the temperature range from 80K-425 K.

Polymer Nanocomposites Made with Unmodified Graphite or Carbon Nanotubes: Role of Dispersion in Optimizing Mechanical and Thermal Properties and Electrical Conductivity

JUNICHI MASUDA, KATSUYUKI WAKABAYASHI, PHILIP BRUNNER, CYNTHIA PIERRE, JOHN TORKELSON, Northwestern University — Polymer nanocomposites made with carbon-based nanofiller have the potential to achieve unprecedented, multifunctional property enhancements in comparison with other nanocomposite systems. Here, we describe research in which we prepare nanocomposites with polymers that are not amenable to solution-based processing, such as polypyrrole and poly(ethylene terephthalate). Solid-state shear pulverization is used singly or in conjunction with melt processing to obtain well-dispersed polymer/graphite and polymer/carbon nanotube nanocomposites. We report record improvements in properties of unoriented films of polypyrrole nanocomposites, including Young’s modulus, crystallization rate, and thermal degradation temperature. We also characterize electrical conductivity of such nanocomposites and note that the dispersion characteristics necessary to achieve maximum mechanical and thermal properties differ from those needed to maximize electrical conductivity. The potential of and challenges with using unmodified graphite as a filler in polymer nanocomposites will be discussed.

Conductive Paper by LBL Assembly of PSS and ITO onto Wood Fibers and its Electrical Properties through Impedance Spectroscopy and I-AFM

CHUNQING PENG, YONATHAN THIO, ROSARIO GERHARDT, Georgia Institute of Technology — Conductive paper has been fabricated by layer-by-layer (LBL) assembly of polyelectrolytes and indium tin oxide (ITO) nanoparticles onto wood fibers, followed by traditional paper making method. The wood fibers were first coated with polyelectrolymeinime (PEI) and then LBL assembled with poly(sodium 4-styrenesulfonate) (PSS) and ITO for several bilayers. The AC electrical properties, measured for frequencies ranging from 0.01 Hz to 1 MHz, will be reported for the in-plane (IP) and through-the-thickness (TT) directions. With 10 bilayers of PSS/ITO assembly on wood fibers, the conductivity of as-prepared paper was improved by more than six orders of magnitude and reach to 5.2×10⁻⁸ S cm⁻¹ in IP direction and 1.9×10⁻⁸ S cm⁻¹ in TT direction. The percolation phenomenon of ITO nanoparticles through the handsheet in both directions was observed through current atomic force microscopy (I-AFM). By applying a bias voltage, either on one end of the paper stripes or on one side of the paper handsheet, the current can be detected on the other end of the paper stripes or on the other side of the paper handsheet. PEI can be used to modify the ITO suspension and significantly improve the LBL procedure. The mechanism of PEI modifying ITO colloidal suspension will be discussed.

Placement Control of Nanomaterial Arrays on Surface-Reconstructed Block Copolymer Thin Films

JEONG GON SON, WAN KI BAE, Seoul National University, HUIMAN KANG, PAUL F. NEALEY, University of Wisconsin-Madison, KOOKHEON CHAR, Seoul National University — Nanomaterials such as nanoparticles, quantum dots and nanorods/wires have recently attracted considerable attention not only because of their unique electronic, optical, and magnetic properties depending on their size and chemical structure but also due to their possible applications to optoelectronic devices, next-generation memory devices, and biological sensors. In order to take full advantage of these useful properties for highly integrated fabrication, precise control of such nanomaterials on patterned substrates is inevitably required. In this presentation, we demonstrate a straightforward and reproducible method for the placement of nanomaterials such as nanoparticles and nanorods on patterned PS-b-PMM block copolymer (BCP) thin films. This concept is based on the properties of surface-reconstructed BCP thin films, which could induce topographical nanopatterns induced by selective solvent vapor treatment without any etching process. The deposition conditions for high density nanomaterial patterns in the grooves of BCP nanopatterns were optimized. By treating the surface under electron beam irradiation, the pattern inversion of nanomaterial-containing BCP nanopatterns was also observed, which can be further processed to realize the dual nanomaterial patterning.

Confinement and Ordering of Au Nanorods in Polymer Films

MICHAEL J. A. HORE, ERIC MILLS, YU LIU, RUSSELL J. COMPOSTO, Department of Materials Science and Engineering, University of Pennsylvania — Ordered arrays of gold nanorods (Au NRs) possess interesting optical properties that might be utilized in future devices. Au NRs functionalized with a poly(ethylene glycol)-thiol brush are incorporated into homopolymer or block copolymer (BCP) films. NR distribution and orientational correlations are studied as a function of nanorod concentration and spacial confinement via Rutherford backscattering spectrometry (RBS) and transmission electron microscopy, respectively. In particular, differences in the degree of nanorod ordering are presented for PMMA homopolymer films (d ~ 45 nm) versus PS-b-PMM block copolymer films (L/2 ~ 40 nm), where higher ordering is seen in the case of BCP films. At moderate volume fractions of NRs, φ = 1% to 10%, the degree of ordering is moderate, and increases with increasing φ. However, coexistence between regions of higher ordering and isotropic orientations is observed. In addition to the planar confinement considered above, orientation of Au NRs confined to cylindrical P2VP domains is studied in PS-b-P2VP BCP films.

Carbon nanotubes nucleate the growth of graphitic layers during carbonization.of electrospun poly(acrylonitrile) nanofibers.

SABINA PRILUTSKY, YACHIN COHEN, EYAL ZUSSMAN, Technion, Israel — Hybrid nanofibers with varying concentration of multwall carbon nanotubes (MWCNTs) in polyacrylonitrile (PAN) were fabricated using the electrospinning technique and subsequently carbonized. The morphology of the fabricated carbon nanofibers (CNFs) at different stages of the carbonization process was characterized by high-resolution transmission electron microscopy (HRTEM) and Raman spectroscopy. In-situ morphological changes during heating were followed by HRTEM using a heated stage. The polycrystalline nature of the CNFs was shown, with increasing content of ordered crystalline regions having enhanced orientation with increasing content of MWCNTs. The results indicate that MWCNTs embedded within the PAN nanofibers nucleate the growth of graphitic layers during PAN carbonization.
10:36AM P19.00014 Crystallization and melting behavior of isatoic polypropylene and carbon nanotube nanocomposites1, GEORGI GEORGIEV, Assumption College/Tufts University, YANIEL CABRERA, LAUREN WIELGUS, Tufts University, ZARNAB IFTIKHAR, MICHAEL MATTERA, PETER GATI, AUSTIN POTTER, Assumption College, PEGGY CEBE, Tufts University, TUFTS/ASSUMPTION COLLABORATION — Polymer nanocomposites(PNCs) are the most recent development in the field of polymer science and technology. Geared toward creating novel polymer based materials, PNCs are the largest commercial application for nanotubes. Spherulitic polymer crystal growth was changed by using new fibrillar crystals on the surface of carbon nanotubes. Upon isothermal melt crystallization at 135°C, CNTs lead to monocrystalline crystal growth perpendicularly to the long axis of the nanotubes, explained by the multiple nucleation centers formed at the interface of the carbon nanotube and the polymer chains. Using Microscopic Transmission Ellipsometry (MTE), the sign of the alpha crystallographic phase was determined as positive. Using Differential Scanning Calorimetry (DSC), a decrease in the Avrami exponent was measured with increase of concentration of nanotubes.

1 Research supported by: the NASA, Programs Program of the DMR, grant (DMR-0602473) and NASA grant (NAG8-1167).

10:48AM P19.00015 Crystallization kinetics in poly(ethylene oxide) / layered silicates nanocomposites, ELENI PAVLOPOULOU, SAPFO FOTIADOU1, ELENI PAPANANOU1, KIIRARI CHRISSOPOLOU, SPIROS H. ANASTASIADIS, Foundation for Research and Technology-Hellas and University of Crete, Heraklion Crete, Greece, GIUSEPPE PORTALE, WIFI BRAS, ESRF-DUBBLE, Grenoble, France — We investigate the effect of inorganic clay on the crystalline characteristics and the crystallization kinetics of PEO in its intercalated nanocomposites with natural montmorillonite (Na+ + MMT). The structure of the hybrids was investigated over multiple length scales by X-ray diffraction, small-angle X-ray scattering (SAXS) and polarizing optical microscopy (POM) as well as by DSC. The PEO within the galleries is completely amorphous whereas only the excess polymer outside the completely full galleries can crystallize at high PEO concentrations. The time resolved measurements reveal the effect of clay on crystallization. Even very small amount of the inorganic can cause a significant decrease of the spherulite size. The crystallization mechanism varies from sporadic nucleation for pure PEO to two-dimensional growth with predetermined nuclei at 10wt% clay with a higher activation barrier for low clay concentration. Sponsored by NATO’s Scientific Affairs Division, by the Greek GSRT and by the EU.

Also at Aristotle Univ. of Thessaloniki, Thessaloniki, Greece

Wednesday, March 18, 2009 8:00AM - 10:48AM
Session P20 DPOLY: Melts and Solutions 321

8:00AM P20.00001 Dynamics and rheology of high molar mass polyethylene oxide solutions, ABHISHEK SHETTY, MICHAEL SOLOMON, University of Michigan — We report dynamic light scattering (DLS), bulk rheology and turbulent drag reduction (TDR) measurements that investigate the structure and dynamics of high molar mass PEO solutions. Steady shear rheology of high molar mass PEO solutions, when modeled by the FENE-P constitutive equation, was consistent with viscoelastic relaxation times much larger than predicted by single polymer, dilute solution theory. DLS of conjugate PEO solutions showed a single relaxation mode in the decay time distribution, which scales as q−2 rather than the q−4 scaling expected of diffusive dynamics. We interpret this result as consistent with the internal dynamics of large multichain domains, clusters or aggregates in the high molar mass PEO solutions. By means of DLS, we also show that the aggregation state of dilute solutions of high molar mass PEO can be manipulated by addition of the chaotropic salt guanidine sulfate or the divalent salt magnesium sulfate. Addition of these salts shifts the power law scaling of the relaxation time from q−4 to q−2. This shift of relaxation time scaling from one indicative of aggregate dynamics (q−4) to one characteristic of polymer center-of-mass diffusion (q−2) shows that these salts are effective de-aggregation agents for PEO. We discuss the results in light of the potential connection between aggregation behavior and polymer TDR of high molar mass PEO.

8:12AM P20.00002 Diffusive Properties of Dilute HPC Solutions: Comparative Study with DLS and FPR, RYAN MCDONOUGH, KIRIL STRELETZKY, Cleveland State University, PAUL RUSSO, Louisiana State University — The dynamics of HPC (Hydroxy-propyl-cellulose) solutions were studied by two fundamentally different methods: FPR (Fluorescence Photo-bleaching and Recovery) and DLS (Dynamic Light Scattering). FPR captures diffusive processes by establishing a photo-bleached boundary and “seeing” only tagged particles diffusing back into bleached area, which yields a contrast function. DLS auto-correlates scattered light intensity from particles in order to determine a statistical decay function. (Dynamic Light Scattering). FPR captures diffusive processes by establishing a photo-bleached boundary and “seeing” only tagged particles diffusing back into bleached area, which yields a contrast function. DLS auto-correlates scattered light intensity from particles in order to determine a statistical decay function. Inverse Laplace transform (CONTIN) and stretch exponential line shape analysis (LSA) serve to quantitatively decompose decay data into different diffusion processes or modes. The first finding is that the CONTIN and LSA results on the same sample are fairly consistent. The second finding is that the modal distributions for FPR and DLS spectra on the same sample show consistent dissimilarities. This indicates a comparative limitation or sensitivity in range of detectable diffusive processes between FPR and DLS in a complex system. The third finding is that the fluorescent tag and tagging process seem to alter the diffusion processes seen by DLS in a way that is consistent; there is a slower mode apparent in non-tagged sample which does not appear in the tagged sample.

8:24AM P20.00003 Helix formation via kinetic assembly of charged block copolymer cylinders in solution, SHENG ZHONG, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware, KE ZHANG, KAREN WOOLEY, Center for Materials Innovation, Department of Chemistry and Department of Radiology, Washington University in Saint Louis, DARRIN POCHAN, Department of Materials Science and Engineering and Delaware Biotechnology Institute, University of Delaware — A multi-micrometer-long, cylinder with helical superstructure is created from coassembly of polyanion (poly(acrylic acid))-block- poly(methyl acrylate)-block-poly(styrene) (PAA-b-PMA-b-PS) triblock copolymers with excessive triethylentetramine or diethylenetriamine in the mixture of 67% volume ratio of water in tetrahydrofuran (THF). The stable pitch distance of the formed helices is due to the balance of long range electrostatic association and uniaxial tension along the cylinder, which can be efficiently tuned by varying the type and amount of the multivalent amine molecules. Double and triple helices are also formed with characteristic interhelical cylinder distances similar to what is observed as the pitch in single helices. A kinetic study shows that the formation of a helix undergoes a complex, but reproducible, nanostructure evolution, including a starting stacked structure, a transition state of very short helices with the length of tens of nanometers and a final multi-micrometer-long mature helix by connecting those short helices.

8:36AM P20.00004 Enhancing Polymer-Fullerene Miscibility Through Enthalpic Interactions, KATIE CAMPBELL, DAVID BUCKNALL, YONATHAN THIO, HASKELL BECKHAM, UWE BUNZ, ADAM HANNON, ANDREW ZAPPAS, BILGE HATLIOGLU, Georgia Institute of Technology, MICHAEL KEMPF, Universität Karlsruhe — Using both theoretical and experimental methods, the use of functional groups in controlling the miscibility between various polymers and fullerenes has been investigated. Molecular dynamics simulations with unmodified C60 and C60 dimers indicated that the number and connectivity of phenyl rings as functional groups, polymer backbone spacing, and aromaticity are all factors in fullerene miscibility. To distinguish between entropic and enthalpic factors, UV-visible spectroscopy was used to determine fullerene solubility with a variety of solvents and also observed changes in solvation concentrations with solvents and polymers. A distinct time dependency for complex formation with many of the fullerene-organic materials investigated was observed as evidenced by a change in solution color with time. Stern-Volmer approximations and fluorescence quenching were used to examine the association of C60 with a series of poly(para-phenylene ethynylene), cyclic polystyrene (PS), and linear PS. The fluorescence quenching of these materials by C60 indicates an association between C60 and the polymer. WAXS studies have shown the formation of C60 aggregates in PS at concentrations of C60 as low as 1 wt%.
8:48AM P20.00005 Modeling Thermodynamic Behavior of Nonionic Surfactants in Water
VALERIY GINZBURG, PIERRE VARINEAU, Dow Chemical Company — Aqueous solutions of nonionic surfactants exhibit a non-trivial phase behavior known as lower critical solution temperature (UCST), where solutions are homogeneous at lower temperatures but become cloudy (two-phase) at higher temperatures. Conventional Flory-Huggins theory of polymer solutions fails to describe such phase behavior. We utilize the approach suggested by Dormidontova and modify Flory-Huggins theory by explicitly accounting for water-water and water-alkylene oxide hydrogen bonding. While the Dormidontova model was restricted to aqueous solutions of polyethylene oxide (PEO), we extend it to include other monomers and their copolymers. With the new approach, we can semi-quantitatively predict cloud points of various nonionic surfactants (TergitolTM and EcosurfTM series) as functions of their molecular structures. We also discuss extensions of this model to calculate micellar phase behavior and oil/water/surfactant interfacial tensions. TM Trademark of The Dow Chemical Company


9:00AM P20.00006 Role of surfactants on the assembly of amphiphilic copolymers through instabilities of organic/water interfaces , JINTAO ZHU, RYAN C. HAYWARD, Department of Polymer Science & Engineering, University of Massachusetts Amherst — We have studied the influence of aqueous surfactants on the assembly of amphiphilic copolymers through hydrodynamic instabilities of organic/water interfaces. Micropipette aspiration measurements on evaporating chloroform droplets containing polystyrene-poly(ethylene oxide) (PS-PEO) diblock copolymers revealed that the onset of interfacial instability and subsequent growth in surface area corresponded to a near vanishing of the interfacial tension. By adding another surfactant, such as sodium dodecyl sulfate (SDS), to the aqueous phase, the chloroform/water interfacial tension was reduced and the onset of instability shifted to lower concentration of PS-PEO. Varying amounts of SDS also led to qualitatively different mechanisms of growth in interfacial area and correspondingly different morphologies of the resulting copolymer assemblies.

9:12AM P20.00007 Influence of Intermolecular Interactions on Fragility of Polymers , KUMAR KUNAL, ALEXEI SOKOLOV, The University of Akron — Glass transition in polymers is a result of slowing down of segmental relaxation. Steepness of the temperature-dependence of segmental relaxation times close to the glass transition temperature, Tg, is expressed in terms of fragility parameter. A strongly non-Arrhenius temperature dependence of segmental relaxation times with steep variations close to Tg is called a ‘fragile’ behavior, and a nearly Arrhenius behavior is called ‘strong’. The existing theoretical models and experimental investigations on polymers with weak van der Waals interactions suggest that fragile behavior of polymers may be linked to their poor packing ability. However, the effect of strong intermolecular interactions on fragility such as polar interactions and hydrogen bonds remains unexplored. It has been predicted that polymers composed of polar monomers are likely to be highly fragile. We have studied polymers with strongly polar interactions and hydrogen bonds and found that although polar polymers do seem to have a higher Tg than their non-polar counterparts, no such conclusion can be drawn about their fragility. The different effects of polar interactions on different classes of polymers may be attributed to the difference in their Tgs.

9:24AM P20.00008 Random Walk of Chain Molecules Along Pore Axis , GUIDUK YU, School of Chem. and Bio. Eng., Seoul National University, SERGEI OBUKHOV, Dpt. of Physics, University of Florida, JIUN-TAI CHEN, Dpt. of Polym. Sci. and Eng., University of Massachusetts Amherst, JUNE HUH, School of Mater. Sci. and Eng., Seoul National University, YOONTAE HWANG, SOONCHUN MOK, School of Chem. and Bio. Eng., Seoul National University, PRIYANKA DOBRIYAL, Dpt. of Polym. Sci. and Eng., University of Massachusetts Amherst, PAPPANNAN THIYAGARAJAN, Intense Pulsed Neutron Source Division, Argonne National Laboratory, THOMAS P. RUSSELL*, Dpt. of Polym. Sci. and Eng., University of Massachusetts Amherst, KYU.SOON SHIN*, School of Chem. and Bio. Eng., Seoul National University — We investigated the overall conformation of polymer chain in cylindrical nanopores using small-angle neutron scattering. The mixture of hydrogenous PS and deuterated PS is confined in nanopores. Surprisingly, the overall conformation of polymer chains along the pore axis is observed to be the same as that in bulk. Even though the chain dimension is larger than the radius of the pores, the chains along the pore axis are not stretched, but sustain to be in unperturbed state. The SANS results implicate that the interpenetration of polymer chains decreases as polymer enters nanopores. We expect the reduction of intermolecular entanglement possibly alters other physical properties of polymer under nanoconfinement.

9:36AM P20.00009 Dynamics of Cyclic Molecules Threaded into a Linear Polymer Chain, KOICHI MAYUMI, HITOSHI ENDO, The University of Tokyo, MICHlHIRO NAGAO, Indiana University and National Institute of Standards and Technology, NOBORU OSAKA, HIDEAKI YOKOYAMA, MITSUHIRO SHIBAYAMA, KOHZO ITO, The University of Tokyo — Dynamics of polynotaxane (PR), in which cyclic molecules, cyclodextrins (CDs), are threaded on an axis linear polymer chain, poly(ethylene glycol) (PEG), are first studied by contrast variation neutron spin echo (CV-NSE). By comparing PRs of hydrogenated and deuterated PEG with different scattering contrasts, we successfully extract two diffusive modes of CDs, corresponding to self diffusion and relative motion to the axis PEG in PR. The self-diffusion constant of CD in PR is determined to be about one-third of the free one in the absence of the axis polymer, which would reflect the space dimension of diffusion with the topological restriction on the axis chain path.

9:48AM P20.00010 Diffusion of Water through Methyl- and Hydroxyl-Terminated Poly(Dimethyldisiloxane)1 , AHMED E. ISMAIL, GARY S. GREST, DAVID R. HEINE2, MARK J. STEVENS, Sandia National Laboratories, MESFIN TSIGE, Southern Illinois University — Both experimental and numerical reports of the diffusion constant of water through poly(dimethylsiloxane) (PDMS) show variances of nearly an order of magnitude. We use molecular dynamics simulations to calculate the diffusion constant for both methyl- and hydroxyl-terminated PDMS chains. We examine the effects of both concentration and chain length. For a single water molecule, we find that diffusion depends strongly on the initial location of the molecule, as the “caging” phenomenon reported by Miller-Plattee can occur. At intermediate concentrations, we observe the formation of dimer and trimer water clusters, leading to lower diffusion rates; at concentrations above the reported aggregation limit of 0.1 wt %, we observe the onset of phase segregation.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.
2Present address: Corning
10:00AM P20.00011 Effect of Stereochemistry and Polydispersity on Diffusion in Polypropylene\textsuperscript{1}. ERNST VON MEERWALL, NUMAN WAHED, WAYNE MATTICE, Univ. Akron — We have performed dynamic Monte-Carlo (MC) simulations and pulsed-gradient diffusion (D) experiments to study the effect of stereochemical composition in linear polypropylene (PP) melts. The coarse-grained simulations were based on the rotational isomeric state model and Lennard-Jones potentials. For the proton NMR diffusion measurements we obtained three PP specimens of differing molecular weight M and dispersity, with the probability of a meso diad Pm = 0.02 (syndiotactic), 0.23 (atactic), and 0.89 (nearly isotactic). The experiment supplied the fixed conversion between MC steps and real time; no dependence on Pm is expected. Both simulation and M-scaled experiment found D at high Pm several times faster than at low Pm. The constant-M simulation also showed a maximum near Pm = 0.8 due to quenched randomness. To find the source of the remaining disagreement with experiment, new simulations tracked the samples’ Pm, mean M, and polydispersity, producing modest improvement. We suspect that the GPC determination of M and its distribution, based on linear polyethylene calibration, is somewhat dependent on PP stereochemistry (via D), generating misleading results.

\textsuperscript{1}Supported in part by NSF (DMR 04-55117)

10:12AM P20.00012 On chain statistics and entanglement of flexible linear polymer melts. SHI-QING WANG, University of Akron — In this work the chain statistics of most linear flexible polymers have been found to be rather universal, allowing chain entanglement to be depicted with few parameters. We first show, to our surprise, based on the literature data of most familiar linear polymers that (a) at the same number of backbone bonds most linear polymers have comparable coil size and are similarly flexible in spite of widely varying chain thickness and (b) the Kuhn length involves a similar number of backbone bonds. The packing model is found to describe the onset molecular weight Mc obtained from the elastic plateau modulus whereas all other models in the literature fail to provide good correlation. It is chain thickness not stiffness that correlates with Mc for over one hundred flexible linear polymers. On the other hand, other models such as percolation model appear to provide some crude correlation for Mc, to which the packing model does not apply well, where Mc denotes the point of departure in the molecular weight scaling from Rouse like to reptation like. Thus, our analysis clarified the apparent contradiction among the various models.

10:24AM P20.00013 Translational Diffusion in a Confined Polymer Melt. JANET WONG, Department of Mechanical Engineering, Imperial College London, LIANG HONG, Dow Chemical Company, SUNG CHUL BAE, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — At the University of Illinois, a new experimental platform has been developed that combines the surface forces apparatus with spatially-resolved fluorescence recovery after photobleaching, giving direct measurements of translational diffusion when polymer melts are confined between mica sheets to controlled thicknesses comparable to the size of the molecules themselves. Applying this platform to polydimethylsiloxane (PDMS), we find not only the anticipated dependence on film thickness but also a dependence on the local pressure: when mica sheets are pressed together so that they flatten, the diffusion of chains confined between them depends on the local pressure, being slowest near the center of the contact. The confined chains split into two populations: those that are immobile on the scale of hours, and those whose mobility is close to that of the unperturbed polymer melt.

10:36AM P20.00014 Entangled Polymer Melt Dynamics Studied By Low-Field NMR. FABIAN VACA CHAVEZ, PATRICK HUEBSCH, RONALD ZIRBS, WOLFGANG BINDER, KAY SAULWAECHTER, Martin-Luther-University Halle-Wittenberg — Proton Multiple-Quantum (MQ) NMR is a powerful technique to investigate polymer dynamics due to its sensitivity to molecular motions on very different timescales. Entangled melts exhibit dynamic processes that cover a wide range of timescales, starting from fast ps-scale segmental reorientation up to diffusive and cooperative motions on the ms-scale. In this work, we apply MQ NMR to linear poly(cis-1,4-isoprene) and poly(isobutylene) of different molecular weight to establish the dynamic regimes predicted by the tube model, and, for the first time, to extract actual time scale information. This directly complements many neutron scattering studies, which are restricted to the sub-\(\mu\)s-timescale. Measurements on PIB-grafted silica particles with different molecular weights and different chain densities on the surface of the particle are also shown. The data is analyzed by establishing scaling laws which can be directly associated with different dynamic regimes predicted by the tube/reptation model. Full analytical analyses based on a correlation function which explicitly includes segmental, Rouse, and reptation dynamics are discussed.

Wednesday, March 18, 2009 8:00AM - 11:00AM –
Session P21 FLAP DCMP: Computational Study of Semiconductor Band Structures 323

8:00AM P21.00001 First-Principles determination of deformation potentials in nitrides. QIMIN YAN, PATRICK RINKE, MATTHIAS SCHEFFLER, CHRIS G. VAN DE WALLE, University of California at Santa Barbara — Group-III nitrides and their alloys are now commonly used in optoelectronic devices such as light emitting diodes (LEDs) and laser diodes (LDs). In these devices strain plays a crucial role since it affects the band structure near the valence- and conduction-band edge and thus the optical properties and the device characteristics. The deformation potentials that describe the change in band structure under strain have not yet been reliably determined, either experimentally and theoretically. Here we present a systematic study of the strain effects in AIN, GaN and InN in the zinc-blende and wurtzite phase. Besides density functional theory (DFT) in the most commonly applied local- and gradient corrected density approximation (LDA/GGA) we also apply the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional \cite{1} and \(G_0W_0\) quasiparticle corrections to address the band gap problem. We present a complete set of deformation potentials that allows us to predict the band positions under realistic strain conditions. For the wurtzite phase we observe non-linearities in the strain dependence that may, in parts, explain the appreciable scatter in previous theoretical work on deformation potentials of group-III-nitrides. \cite{1} J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003) Work supported by the UCSB Solid State Lighting and Energy Center.

8:12AM P21.00002 Band-gap bowing, band offsets, and electron affinity for InGaN alloys: A DFT study.\textsuperscript{1}. POUL MOSES, CHRIS VAN DE WALLE, UCSC — InGaN alloys are successfully being used in optical, electronic, and photovoltaic devices; a novel application is for photochemical water splitting. Because the InGaN alloys using density functional theory. The HSE exchange correlation functional has been used in order to accurately calculate the electronic band structure \cite{1}. Detailed surface calculations have been performed that, combined with bulk calculations for alloys, yield information about the positions of valence and conduction bands on an absolute energy scale. We will discuss bowing effects, band offsets, and electron affinities in light of the application of InGaN alloys for photochemical hydrogen production. \cite{1} J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207 (2003)

\textsuperscript{1}We acknowledges support from ACS-PRF Grant number 47379-AC10
8:24AM P21.00003 A Hybrid Look at Band Offsets in AlN/GaN Heterostructures, JEREMY NICKLAS, JOHN WILKINS — Hybrid functionals have been gaining traction for their better estimation of band gaps in semiconductors. Recently, a screened hybrid functional, HSE, has been introduced that improves upon the hybrid functionals by essentially screening out the Fock exchange after a given radius. This study compares how well the HSE functional does with the technologically important band offsets in the AlN and GaN wide bandgap heterostructures compared to experiment and other previous theoretical calculations. Both the strained polar hexagonal and the nonpolar cubic phases of these III-V semiconductors are taken into consideration. Due to the large induced electric field in the polar hexagonal structure, a multipole decomposition will be discussed as well.

8:36AM P21.00004 Reassessing the Description of the Electronic Structure of a Semiconductor Alloy1, YONG ZHANG, A. MASCARENHAS, National Renewable Energy Laboratory, L.-W. WANG, Lawrence Berkeley National Laboratory — Although an electronic state in an alloy like Ga1-xInxP is not a Bloch state, it is generally considered to be reasonably close to a Bloch state in the sense of a virtual crystal approximation (VCA), and it is often referred to as Γ-like, L-like, or X-like. We have find that within certain context one could call a band edge state as Γ-like, if the dominant component of its wavefunction is indeed the Γ state of the VCA, but globally the alloy states are in general very different from those of the VCA in two important aspects: (1) a Γ-like state, for instance, could in fact have a very small Γ component of the VCA state, and (2) if the corresponding VCA states are degenerate, for instance, a Χ-like band edge alloy state, there will be strong coupling among the degenerate valleys. These new insights have major impacts on our understanding of the optical and electronic properties[1], and the ordering effects [2] in a semiconductor alloy.

1Supported by DOE/BES/DMSE.

8:48AM P21.00005 Ab initio study of the optical properties of Si-XII, BRAD MALONE, JAY SAU, MARVIN COHEN, Department of Physics, University of California, Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We present a first-principles calculation of the optical excitation spectrum of Si-XII, a high-pressure, metastable phase of silicon in the R8 structure. Recent calculations of the quasiparticle spectrum have shown Si-XII to be semiconducting with a small, indirect band gap. In this paper we solve the Bethe-Salpeter equation (BSE) to obtain the optical spectrum of this material. We then compare our calculated optical spectrum with experimental data for other forms of silicon commonly used in photovoltaic devices. These include cubic, polycrystalline, and amorphous forms of silicon. We find that the calculated values of the optical functions relevant to photovoltaic absorption in Si-XII show great overlap with the incident solar spectrum than those found in these other silicon phases.

9:00AM P21.00006 First-Principles Hartree-Fock Study of Locations and Hyperfine Interactions of Transition Metal Impurities in Silicon, R.H. PINK, S.R. BADU, SUNY Albany, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, LEE CHOW, UCF Orlando, M.B. HUANG, T.P. GAS, SUNY Albany — The study of the magnetic properties of transition metal ions in silicon is currently of great interest because of their potential applications in spintronics. An understanding of the ferromagnetism associated with the interactions between these impurities requires a knowledge of their locations in the lattice. Three possible locations of Mn2+, V2+, and Cr3+ ions have been investigated, namely, the interstitial hexagonal (H) and tetrahedral (T) and substitutional (S) sites. Both binding energies and hyperfine interactions are being studied using the Hartree-Fock Cluster procedure with many-body effects included by the many-body perturbation theory (MBPT) procedure. For Mn2+ ion, the Hi site is found to be unstable while the Ti and S sites have positive binding energies. Our calculated 55Mn hyperfine constant favors the Ti site which is also supported by channeling measurements.

2J. LalRose and M.B. Huang (to be published).

9:12AM P21.00007 Theoretical analysis of the effect of tip-induced band bending on scanning tunneling spectroscopy measurements on H-terminated Si(100) surface, HIDEOMI TOTSUKA, totsuka.hideomi@nihon-u.ac.jp, SATOSHI WATANABE, watanabe@cello.t.u-tokyo.ac.jp — Scanning tunneling spectroscopy (STS) is widely used experimental technique. However, theoretical study on STS is not sufficient yet, in the sense that the effects of important factors such as the tip-induced band bending (TIBB) in measurements on semiconductor surfaces have not been examined yet. In this study, we have analyzed the STS spectra on a H-terminated Si(100) surface theoretically using a method [1] which can calculate the electron states under applied bias voltages self-consistently. We found that the band gap in the STS spectra is larger than that in the density of states calculation. Furthermore, we found that this cannot be understood from TIBB, while the bias voltage dependence of TIBB in our calculation corresponds well with experimental result [2]. [1] Y. Gohda et al., Phys. Rev. Lett. 85, 1750 (2000). [2] M. McEllistrem, et al., Phys. Rev. Lett. 70, 2471 (1993)

9:24AM P21.00008 Band gaps and band offsets in the SiO2/Si interface calculated by including the self-energy of electrons and holes, LUIZ FERREIRA, Universidade de São Paulo, Brazil, LEONARDO FONSECA, MAURO RIBEIRO, Jr., Center Werner von Braun for Advanced Research, Brazil — Density Functional theory, as formulated by Kohn and Sham (Phys. Rev. 140, A1133 (1965)), is insufficient when it comes to the calculation of one-particle excitations (electrons and holes). In this case, one has to include the self-energy of the particle (see for instance R. Gómez- Abal. et al Phys. Rev. Lett. 101, 106404 (2008)). This self-energy is mostly the classical electrostatic self-energy of the particle charge density but has an important contribution from exchange and correlation. In a recent paper (L. G. Ferreira et al, Phys. Rev. B 78, 125116 (2008)), it is shown that the self-energy can be calculated with the help of a “self-energy potential”, wholly derived from pure atomic calculations. The band gaps calculated with those self-energies are precise, in no way worse than the GW band gaps, and yet the calculation is very simple and fast. Next challenge we faced was the calculation of the band-offsets of the all important Si/SiO2 system. Notice that the “self-energy potential” is centered between two covalent bonded atoms in the Si side and centered at the O in the SiO2 side. Then the question is whether these self-energy potential perturbations create a wrong charge density at the interface. The answer is that both gaps and band offsets were calculated with outstanding quality.
9:36AM P21.00009 The influence of pressure on defects in amorphous silicon1. JEFFREY GROSSMAN, LUCAS WAGNER, University of California, Berkeley — Amorphous silicon(a-Si) thin-film solar cells are promising materials for solar cells, but they suffer from the Staebler-Wronski effect (SWE), in which the efficiency degrades over the course of a few hours of light exposure. While there has been progress in mitigating this effect through sample preparation, there is still no clear microscopic explanation for the degradation. We have used first principles density functional theory and highly accurate quantum Monte Carlo calculations to investigate the effect of pressure on different types of defects present in a-Si. Our calculations show that the effect of pressure on a-Si is strongly dependent on the particular type of defect, and they further may provide new ways to experimentally determine the dominant defect type. We also report on the effect of pressure on the simplest reaction in a-Si: a bond switch between two neighboring Si atoms, which could be an important element in the understanding of the SWE [1]. [1] L. K. Wagner and J. C. Grossman. PRL (in press)

1Supported by the NSF and the Center for Integrated Nanomechanical Systems.

9:48AM P21.00010 Ab initio calculations of the dielectric functions of semiconductors and alloys including excitonic effect via LASTO method. HYEJUNG KIM, YIA-CHUNG CHANG, Department of Physics, University of Illinois at Urbana-Champaign, Urbana IL and Research center for Applied Sciences, Academia Sinica, Taipei, Taiwan — We calculate dielectric functions of semiconductors and alloys including the electron-hole interactions within the ab initio framework. The Bethe-Salpeter equation is constructed using a full-potential linear augmented-Slater-type orbital (LASTO) method. The electron-hole interaction is computed with a sufficiently dense k-point mesh, which shows good convergence. Point group symmetry has been utilized to speed up the computation significantly. Dielectric functions of alloys are calculated by the configurational average of special quasirandom structures. The inclusion of the electron-hole interaction both shifts the peak positions and changes peak heights of the imaginary part of the dielectric functions, resulting in better agreement with ellipsometry data than the spectra obtained without including the electron-hole interactions.

10:00AM P21.00011 The Electronic and Optical Properties of Manganese-doped Wurtzite ZnO. YIMING MI, XINXIN ZHAO, School of Fundamental Studies, Shanghai University of Engineering Science, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo — The electronic and optical properties of Manganese-doped Wurtzite ZnO were studied by the first principles pseudopotential plane wave method within density functional theory formalism. The electronic structures, density of states, and optical absorption spectra were investigated for different doping concentration. The acquired results reveal that the energy gap of the Mn-doped ZnO increases with the increase of Mn-doping concentration, and the UV absorption of the system gets stronger with the Mn-doping concentration augmented, which are consistent with others’ calculation and experimental results fairly well.


1This work was supported by the Director, Office of Science, Basic Energy Sciences, Division of Material Science and Engineering, and the Advanced Scientific Computing Research Office, of the U.S. Dept. of Energy under Contract No. DE-AC02-05CH11231.

10:24AM P21.00013 Dielectric Function and Critical Point of GeSbTe Pseudo-binary Compound Thin Films. HOSUNG LEE, JUN-WOO PARK, Kyung Hee University, YOUN-SEON KANG, TAE-YON LEE, DONG-SEOK SUH, KI-JOON KIM, CHEOL KYU KIM, YOON HO KANG, Samsung Electronics, JUAREZ L. F. DA SILVA, NREL — We measure the dielectric functions of GeSbTe pseudo-binary thin films by using spectroscopic ellipsometry. We anneal the thin films at various temperatures. According to x-ray diffraction, the as-grown thin films are amorphous and the annealed films have metastable and stable crystalline phases. By using standard critical point model, we obtain the accurate values of the energy gap of the amorphous phase as well as the critical point energies of the crystalline thin films. The critical point energies are compared to the band gap energies determined by the method of linear extrapolation of the optical absorption. As the Sb to Ge atomic ratio increases, the optical (band) gap energy of amorphous (crystalline) phase decreases. Standard critical point fitting show several higher band gaps. The electronic structures and the dielectric functions of the thin films are calculated by using density functional theory and are compared to the measured ones. The band structure calculations show in stable phase that GeTe, GeSbTe3, and Ge3Sb2Te7 have indirect gap whereas Ge5Sb1Te17 and Sb2Te3 have direct gap. The measured indirect band gap energies match well with the electronic band structure calculations.

10:36AM P21.00014 Origin of the unusually large band gap bowing and the breakdown of the band-edge distribution rule in the SnxGe1-x alloys. WAN-JIAN YIN, XIN-GAO GONG, Fudan University, Shanghai, China, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado, USA — Most semiconductor alloy AxB1-x has a non-linear dependence of its band-edge distribution rule in the SnxGe1-x alloys. The bowing parameter is the band-gap difference between the direct interband transition of a system and the so-called bowing parameter, which is the average of two valence band edge states and find that the bowing of the conduction band edge is much larger than the bowing of the valence band edge, although the natural valence band offset between Ge and Sn is larger than the natural conduction band offset. The breakdown of the band-edge distribution rule is explained by the large lattice mismatch between Ge and Sn and the large deformation potential of the band edge states.

10:48AM P21.00015 Accurate electronic structure calculations of lead chalcogenides by QSGW method. SERGEY FALEEV, OLEG MYRASOV, Seagate Technology — Enhancement of the energy conversion efficiency of thermoelectric materials has been a long goal of materials physics. Recent experiments show that distortion of the electronic structure of PbTe by adding small amount of impurities results in enhancement of the Seebeck coefficient and doubling of the ZT factor [Heremans et al., Science 321, 554 (2008)]. This enhancement is thought to be due to the impurity-induced increase of the energy dependence of density of states near the Fermi level. The reliable theoretical prediction of the energy states of impurities in host matrix (which often very difficult to measure experimentally) are required in order to explain the experiments and predict and optimize properties of new materials. Accurate calculations for bulk system is a first necessary step required for further study of systems with impurities. Here we report results for bulk lead chalcogenides obtained with recently developed QSGW method [Faleev et al., PRL 93, 126406 (2004)]. We found that electronic structure of lead chalcogenides and, in particular, the band gaps and effective masses are predicted with much higher accuracy within the QSGW approach than within most commonly used DFT theory. This result opens way for predictive search of novel thermoelectric materials.
8:00AM P22.00001 Beller Lectureship Talk: Spin Hall Effect  . MICHEL I. DYAKONOV, University of Montpellier II, CNRS, France — The Spin Hall Effect (SHE) and related transport phenomena originating from the coupling of the charge and spin currents due to spin-orbit interaction were predicted [1] in 1971. Following the suggestion in [2], the first experiments in this domain were done at Joffe Institute in Saint Petersburg [3], providing the first observation of what is now called the Inverse Spin Hall Effect. As to the SHE itself, it had to wait for 33 years before it was experimentally discovered by two groups [4] in Santa Barbara (US) and in Cambridge (UK). The phenomenon consists in spin accumulation at the lateral boundaries of a current-carrying non-magnetic conductor, the spin directions being opposite at the opposing boundaries. The boundary spin polarization is proportional to the current and changes sign when the direction of the current is reversed. It exists in relatively wide spin layers determined by the spin diffusion length, typically on the order of 1 µm. I will discuss the phenomenology of spin-charge coupling, the underlying microscopic mechanisms, and the existing experimental results obtained in semiconductors and metals at cryogenic, as well as at room temperatures. I will also address a related, but as yet unknown phenomenon, the "swapping" of spin currents, which is due to the correlation between spin rotation during a scattering event and the direction of scattering. [1] M.I. Dyakonov and V.I. Perel, JETP Lett. 13, 467 (1971); Phys. Lett. A35, 459 (1971) [2] N.S. Averkiev and M.I. Dyakonov, JETP Lett. 35, 196 (1983) [3] A.A. Bukun et al., JETP Lett. 40, 1293 (1984) [4] Y.K. Kato et al., Science 306, 1910 (2004); J. Wunderlich et al., Phys. Rev. Lett. 94, 047204 (2005)  

8:36AM P22.00002 Spin Hall frequency doubling and spin memristive effects1 . YURI V. PERSHIN, Department of Physics and Astronomy and USC Nanocenter, University of South Carolina, Columbia, South Carolina 29208, USA; MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego, La Jolla, California 92093-0319, USA — It is shown that when a time dependent voltage is applied to a system with inhomogeneous electron density in the direction perpendicular to main current flow, the spin Hall effect results in a transverse voltage containing a double frequency component. We demonstrate that there is a phase shift between applied and transverse voltage oscillations, related to memristive behavior of semiconductor spintronics systems. It is interesting that spin memristive effects in this system are manifested directly in the voltage response. A different method to achieve the second harmonic generation, based on the inverse spin Hall effect, is also discussed.  

1This work was partially supported by the National Science Foundation and Department of Energy.  

8:48AM P22.00003 Enhanced Spin Hall Effect by Single Antidot Potential . MIKIO ETO, TOMOHIRO YOKOYAMA, Faculty of Science and Technology, Keio University — We theoretically investigate an extrinsic spin Hall effect in semiconductor heterostructures due to the scattering by an artificial potential created by a single antidot, STM tip, etc. The strength of the potential is electrically tunable. First, we formulate the spin Hall effect in terms of phase shifts in the partial wave expansion for two-dimensional electron gas. For scattered electrons in θ direction, we obtain a spin polarization P(θ) perpendicular to the two-dimensional plane [P(_−θ) = −P(θ)]. The spin polarization P(θ) is significantly enhanced by an attractive potential when the resonant condition of a partial wave is satisfied by tuning the potential strength. Second, we study the spin Hall effect in a three-terminal device with an antidot at the junction. The conductance and spin polarization are evaluated numerically [1]. We obtain a spin polarization of more than 50% due to the resonant scattering when the attractive potential is properly tuned.  


9:00AM P22.00004 Competing interplay between Rashba and cubic-k Dresselhaus spin-orbit interaction in spin Hall effect1 . C.S. CHU, R.S. CHANG, Dept. of Electrophysics, National Chiao Tung University, Taiwan, ROC, A.G. MAL’SHUKOV, Institute of Spectroscopy, Russian Academy of Science, Russia — We study the interplay between the Rashba and cubic-k Dresselhaus spin-orbit interactions (SOI) in a diffusive two-dimensional electron gas (2DEG). Within the spin Hall configuration, we perform a systematic calculation of the spin accumulation S_i and the spin polarizations S_{ij} at the lateral edges and in the bulk of the 2DEG, respectively. Both the relative coupling strength of the Rashba and the Dresselhaus SOI, and the electron densities are varied. The spin accumulation exhibits strong competing features, including in the Dresselhaus-dominant regime the sign change in S_z when electron density is large enough, and in the Rashba-dominant regime the complete suppression of S_z. Most surprisingly is our finding that the Rashba-dominant regime occurs as early as α ≈ β, where α, β are the Rashba and the effective linear-k Dresselhaus SOI coupling constant, respectively. Similar Rashba-dominant regime is found in the spin polarizations, when α ≥ β. Our results point out that decreasing |α| leads to the restoration of the spin accumulation.  

1Work supported by Taiwan NSC No. 96-2112-M-009-0038-MY3  

9:12AM P22.00005 Monte Carlo Simulation of Spin-Injection Hall Effect . LIVIU P. ZÁRBO, JAIRO SINOVA, Department of Physics, Texas A&M University, USA; JÖRG WUNDERLICH, Hitachi Cambridge Laboratory, United Kingdom; TOMAS JUNGWIRTH, Institute of Physics, ASCR, Czech Republic; SHOU-CHENG ZHANG, Department of Physics, Stanford University, USA — The spin-injection Hall effect, which is the newest addition to the spintronic Hall effect family, consists in the transversal deflection of a charge spin-polarized current injected in a spin-orbit coupled semiconductor channel which results in transverse Hall voltage whose magnitude varies along the channel direction. Just as in the case of spin Hall effect, the phenomenon is due to both intrinsic and extrinsic (impurity driven) spin-orbit scattering. We develop a semiclassical spin-dependent Monte Carlo simulation technique which enables us to quantitatively explain the mechanisms of spin-injection Hall effect in experimentally relevant systems. This is achieved by incorporating both intrinsic and extrinsic contributions to anomalous Hall effect (AHE) which are rigorously derived within the recently developed gauge invariant semiclassical theory of AHE. The advantage of this approach over a fully quantum mechanical treatment is that it enables us to investigate the spin-injection Hall effect in micrometer-size devices while still retaining the essential physics.  

9:24AM P22.00006 Calculations of Spin-orbit Splittings in Two-Dimensional Heterostructures1 . MARTA PRADA, MARK FRIESEN, ROBERT JOYNT, University of Wisconsin-Madison, QUANTUM COMPUTING GROUP TEAM — We present calculations of spin-orbit level splittings in GaAs/InGaAs and Si/SiGe quantum wells. We use both an effective mass approach and a numerical tight-binding approach (NEMO-3D) that includes the effects of the interfaces on atomic scales. We are able to separate the Rashba and Dresselhaus contributions. The calculations are done as a function of applied electric field and well width. We find good agreement of theory and experiment for the measurements of L. Meier et al., (Nature Physics 3, 650 (2007)) on GaAs/InGaAs. In Si/SiGe wells, we find significant valley- spin-orbit mixing and also that the Dresselhaus term is substantial, and can even be larger than the Rashba term for realistic parameters.  

1Spanish Ministry of Education and Science, NSF-ITR 0325634 and NSF-EMT 0523680
9:36AM P22.00007 Coherent ultrafast spin flip in a 2D electron gas\textsuperscript{1}. CAREY PHEILPS, TIMOTHY SWEENEY, HAILIN WANG. Department of Physics and Oregon Center for Optics, University of Oregon, Eugene, OR 97405 — We report the experimental demonstration of ultrafast electron spin flip in a modulation doped CdTe quantum well. Complete spin flip is realized with an off-resonant laser pulse of 2 ps in duration. The effective pi-pulse flips the electron spins with respect to an axis that is orthogonal to both the external magnetic field (Voigt geometry) and the sample growth axis. The realization of the ultrafast pi-pulse opens up a new avenue for protecting electron spins from decoherence with dynamical decoupling.

\textsuperscript{1}This work is supported by NSF and ARL.

9:48AM P22.00008 Analysis of Electron Spin Relaxation Momentum Time in Narrow Gap Semiconductor Quantum Well and Dots: Including Rashba and Dresselhaus Effects. YUNG-SHENG HUANG, JUNG-SHENG HUANG, College of EECS, Semiconductors Research Laboratory, I-Shou Univ., 840 Kaoshuing, Taiwan — A model of GaAs quantum dots embedded in a quantum wire is studied. We want to investigate how the electron spin relaxation momentum time (SRT) is varying with some physical parameters. We find that SRT decreases while the four parameters, external magnetic field, surrounding temperatures, both quantum wire width and thickness increase. The reason is caused by more and more phonons resulted in a higher scattering probability between electrons and phonons. Thus the SRT is reduced. Besides, Lommer and Silva showed that in narrow gap semiconductor bulk materials, the Rashba effect is larger than Dresselhaus effect. Our results show that Dresshaus effect is larger than Rashba effect for the quantum well under electric field, especially when the quantum well width is small. The authors are interested in studying whether the same characteristics exist in quantum dots. We are working on this line.

10:00AM P22.00009 Spin accumulation in a Rashba-type two-dimensional electron gas due to a nonuniform driving electric field\textsuperscript{1}. LU-YAO WANG, CHON-SAAR CHU, Department of Electrophysics, National Chiao Tung University, MAL SHUKOV ANATOLY, Institute of Spectroscopy, Russian Academy of Science — It is well understood that a Rashba-type two-dimensional electron gas (2DEG) does not support spin accumulation, or spin Hall effect, in the diffusive regime when the driving electric field is uniform. In this work we address the issue about a possible restoration of the spin Hall effect when the driving field is nonuniform. Toward this end, we consider the spin accumulation in the vicinity of a circular hole, with radius $R \sim l_{so}$, where the driving field becomes nonuniform. Here $l_{so}$ is the spin relaxation length, and $l_{so} \gg l_{c}$, the mean free path. Our result shows that the nonuniform driving field gives rise to nonuniform in-plane spin densities $S_x$ and $S_y$, which in turn contribute to a finite spin current via the combined processes of spin diffusion and spin-precession. The spin accumulation thus obtained is proportional to the Rashba coupling constant $\alpha$, and its spatial pattern is one of spin-dipole form, aligned perpendicular to the driving field.

\textsuperscript{1}Supported by NSC 96-2112-M-009-038-MY3

10:12AM P22.00010 Scattering approach in calculating Rashba Spin-orbit coupling in asymmetric\textsuperscript{1}. CHIH-PIAO CHUU, QIAN NIU — The Rashba Spin-orbit coupling plays a crucial role in spin manipulation in semiconductor heterostructures. We study the underlying physics through scattering approach with the Kane model. Several physical parameters are considered, including potential barrier asymmetries, quantum well inclination, as well as band structure parameters. This may provide a better understanding in designing spintronic devices.

10:24AM P22.00011 2D Holstein polarons in the presence of spin-orbit interactions. LUCIAN COVACI, MONA BERCIU, University of British Columbia, Vancouver, Canada — The electron-phonon interaction in the presence of spin-orbit interactions (of either Rashba or Dresselhaus type) must be taken in account for GaAs quantum dots or for spintronic devices. The possibility of tuning the electron-phonon interaction by coupling to a substrate (e.g. in organic transistors) requires an accurate treatment of this problem in all coupling regimes. We apply a recently developed approximation (the Momentum Average Approximation) to this specific theoretical question. We have shown that this method is exact in various asymptotic regimes while being accurate for all coupling strengths. We calculate the self-energy at the MA(2) level of the approximation. From ground state properties (energy and effective mass) we conclude that in the presence of spin-orbit interactions, the polaron is harder to trap – the crossover from large to small polarons is shifted to higher couplings. From the spectral function, we show that there are two distinct regimes, depending on relation between the phonon frequency and the strength of the spin-orbit interaction. When the latter is larger we find that the polaron character is dominated by only one band (the '-' band). We also show that the off-diagonal part of the self-energy plays an essential role in obtaining the polaron + one phonon continuum correctly.

10:36AM P22.00012 Full spin control in 2DEGs with no magnetic fields. B.J. MOEHLMANN, M. E. FLATTÉ, OSTC and Department of Physics and Astronomy, University of Iowa — A properly chosen closed spin transport path in the plane of a III-V semiconductor quantum well suffices for arbitrary spin manipulation of conduction electrons about any desired axis. This feature of spin transport relies on the non-commutativity of the precession matrices associated with non-colinear path segments. The electron spin rotation depends solely on the path geometry, not the speed of the spin along the path. Simple closed paths have been found which will perform arbitrary spin rotations along arbitrary axes with no net spatial displacement of the spins. The paths differ depending on the form of the internal effective magnetic fields induced by crystal asymmetry, growth asymmetry, and strain and electric fields. This work was supported by an ONR MURI.

10:48AM P22.00013 Many-body effects on $\rho_{xx}$. Ringlike Structures via SDFT\textsuperscript{1}. GERSON J. FERREIRA, HENRIQUE J. P. FREIRE, J. CARLOS EGUES, University of Sao Paulo — In the quantum Hall regime, the longitudinal resistivity $\rho_{xx}$ plotted in a density-magnetic-field diagram displays ringlike structures due to the crossings of spin split Landau levels of distinct subbands. We theoretically investigated the dependence of the magnetoresistance on the magnetic field tilt angle and on the temperature using Spin Density Functional Theory (SDFT). Assuming a temperature dependence of the Landau levels broadening, we show that the ringlike structures are broken at sufficiently low temperatures due to a ferromagnetic quantum phase transition. Additionally, for tilt magnetic field, the momentum in the growth direction (z) also couples to the magnetic field $z P_{\perp}$ coupling, thus giving rise to anticrossings between consecutive Landau levels and subbands, collapsing the ring with increasing tilt angle. We find that the interplay of these anticrossings and many-body interactions (via SDFT) leads to a reduced $z P_{\perp}$ coupling, increasing the collapsing angle at which the ring fully disappears. Our results explain some of the physical mechanisms behind ring formation and collapse which have been experimentally observed.

\textsuperscript{1}We acknowledge support from FAPESP and CNPq.
8:00AM P23.00001 Temperature dependence of the phonon density of states in FeSi and CoSi, OLIVIER DELAIRE, Oak Ridge National Laboratory, MATTHEW LUCAS, MATTHEW STONE, DOUGLAS ABERNATHY — The phonon density of states (DOS) of the B20 compounds Fe(1-x)Co(x)-Si (x=0.0, 0.03, 0.5, 1.0) was measured as a function of temperature from 10K to 773K using inelastic neutron scattering. The phonon DOS of FeSi exhibits an excess softening compared to the predictions of the quasiharmonic model, in agreement with previous measurements of elastic constants as function of temperature [1]. The phonon DOS of CoSi softens less, on the other hand, and appears in better agreement with the pure volume effect of the quasiharmonic model. These trends are compared to previous measurements of the temperature dependence of the phonon DOS in the A15 compounds V5Si3 and V3Ge [2]. Using first-principles electronic structure calculations, the observed anomalies are related to the details of the band structure in these compounds. It is shown that sharp features in proximity to the Fermi level lead to anomalous phonons through a sensitivity to thermal disorder, or adiabatic electron-phonon coupling. [1] D. Mandrus et al., Phys. Rev. B 51, 4763 (1994) [2] O. Delaire et al., Phys. Rev. Lett. 101, 105504 (2008)

8:12AM P23.00002 Effects of temperature and chemical order on phonons in Fe-V alloys, MATTHEW LUCAS, Oak Ridge National Lab, JORGE MUNOZ, California Institute of Technology, OLIVIER DELAIRE, Oak Ridge National Lab, BRENT Fultz, California Institute of Technology, DOUGLAS ABERNATHY, MATTHEW STONE, MARK LOGUILLIO, Oak Ridge National Lab — Inelastic neutron-scattering spectra were measured on body-centered-cubic Fe-V alloys as a function of temperature and composition. These data were reduced from time-of-flight histograms to spectra that resemble the phonon density of states (DOS), but were distorted by differences in efficiencies of the atom species for phonon scattering. Nuclear resonant inelastic x-ray scattering spectra were measured for the 57-Fe isotope in a similar set of alloys at room temperature to compliment the neutron spectra. With temperature the 50-50 alloy undergoes an ordering transition from A2 to B2, as evidenced by increasing intensity in the superlattice peaks from the elastic regime of the neutron spectra. This ordering is accompanied by a change in the phonon DOS. The Connolly-Williams cluster inversion method is performed on the DOS of the disordered Fe-V alloys in order to correlate changes in the chemical order with changes in the DOS for the 50-50 alloy. The temperature dependence of the DOS of the disordered alloys is used to determine the anharmonic phonon entropy, and the chemical dependence to determine the phonon entropy of mixing.

8:24AM P23.00003 Ambipolar diffusion and recombination of photoexcited carriers in bismuth films, YU-MIIN SHEU, YI-JIUNN CHIEN, CITRAD UHER, STEPHEN FAHY, DAVID REIS, FOCUS Center and Department of Physics, University of Michigan, Ann Arbor, Michigan 48109-1040, USA — Recent experimental and theoretical studies on bismuth show that intense ultrafast photoexcitation leads to a large−amplitude, softened coherent Alg phonon. Thus, the subsequent dynamics of the photoexcited carriers will strongly influence the dynamics of the phonon. However, little is known about the nonequilibrium carrier dynamics due to difficulty in separating carrier relaxation and other processes. Here we report ultrafast counter propagating pump-probe experiments, measuring photoexcited carrier transport across optically thick single crystal bismuth films at room temperature. The films are grown on transparent sapphire substrates with thicknesses varying between 185 and 385 nm, sufficient to separate the carriers from the effects of lattice heating and strain, when pumped and probed on opposite faces. The measured recombination time is about 14-30 ps and the carrier recombination time is much longer than the Alg phonon period, supporting a two chemical potential model for the photoexcited electronic system and phonon dynamics, in which carrier diffusion (rather than electron-hole plasma cooling or recombination substantially reduces the carrier density over the lifetime of the phonon, leading to a chirped mode.

8:36AM P23.00004 Magnetotransport in ultra quantum Bismuth and related alloys, DORON BERGMAN, KARYN LE HUR, Yale University — Recent studies of elementary Bismuth and related alloys in strong magnetic fields, have uncovered peculiar electric and thermal transport behavior (Bhnia et al. Science 317, 1729 (2007), Banerjee PRB 78, 161103 (2008)). In particular, the Hall resistivity resembles that of the fractional quantum Hall effect, in exhibiting quasi-plateaux, corresponding to fractional filling factors. At the same time anomalous features appear in the Nernst and Seebeck coefficients. Recent efforts to address possible interaction effects (Burnell et al., Aicel et al. preprints 2008), while suggesting interesting electronic states of Bismuth in this ultra quantum regime, have not explained the unusual transport phenomena. We investigate the transport phenomena in more detail, by using a microscopic model of the Bismuth band structure. We first explore Landau level physics in this model, and then go on to develop a theory of the anomalous transport phenomena, using Boltzmann kinetic theory.

8:48AM P23.00005 Angular dependent Nernst effect in Bi,Sb, across the quantum limit, KAMRAN BEHNIA, ZENGWEI ZHU, BENJOUT FAQUÉ, ARITRA BANERJEE, ESPCL, BERTRAND LENOIR, Ecole des Mines — The Fermi surface of bismuth occupies a tiny (10−5) fraction of the Brillouin zone. Therefore, a field of 9 T oriented along the trigonal axis pushes the electrons to their lowest Landau level. Allowing bismuth with antimony reduces the carrier density and lowers this threshold field known as the quantum limit. Approaching this limit, the Nernst-Ettingshausen effect was found to control the macroscopic quantities whose magnitude is yet to be understood. The Nernst response presents sharp peaks each time a Landau level of hole-like quasi-particles meets the chemical potential. In addition to these peaks, a number of anomalies of unidentified origin were detected. Here, we present the first study of Nernst effect as a function of a rotating magnetic field in Bi,Sb, up to 12 T. The results highlight the role played by the Dirac quasi-particles of the electron pockets in the generation of the unidentified anomalies.

9:00AM P23.00006 Thermal transport properties of two-dimensional Dirac fermion, YOUSSEF ROMIAH, Department of Physics and Texas Center for Superconductivity, University of Houston, XIN-ZHONG YAN, Chinese Academy of Science, CHIN-SEN TING, Department of Physics and Texas Center for Superconductivity, University of Houston — The self consistent Born approximation is utilized to obtain the electronic density of states of the disordered alloys is used to determine the anharmonic phonon entropy, and the chemical dependence to determine the phonon entropy of mixing.

9:12AM P23.00007 Grain coarsening in crystals from evolution of dislocation densities: Results from a continuum theory of dislocation dynamics, WOOSONG CHOI, YONG CHEN, STEFANOS PAPANIKOLOAU, JAMES SETHNA, Cornell University, SURACHATE LINKUMNERD, Chulalongkorn University — Continuum theories of grain growth and coalescence dynamics are used to incorporate dislocation line tension energy, and explore the resulting coarsening mechanisms in two dimensions. We report initial results both on scaling behavior, coarsening and coalescence phenomena in more detail, by using a microscopic model of the Bismuth band structure. We first explore Landau level physics in this model, and then go on to develop a theory of the anomalous transport phenomena, using Boltzmann kinetic theory.

9:24AM P23.00008 Smooth versus jerky motion of packets of dislocations across fields of obstacles. CATALIN PICU, RENGE LI, Rensselaer Polytechnic Institute — We report on the transition from smooth (“unzipping”) to jerky motion of multiple interacting dislocations (elastic manifolds) moving across a field of randomly located obstacles under constant applied stress. The transition is controlled by the stress, the obstacle strength and distribution. The system exhibits spatial and temporal correlations ( intermittency) similar to those observed experimentally at much larger scale in dislocation avalanches. Power law distributions of jump amplitudes and separation times emerge. Comparison of the simulation results with experimental data indicates that the jerky motion is more relevant for plastic deformation of real crystals than unzipping. The strain rate sensitivity parameter, m, decreases sharply when the system enters the jerky mode and becomes independent of the obstacle strength, presence of obstacles of various strengths and the way those are mixed, and of temperature.

9:36AM P23.00009 Molecular-dynamics analysis of the mechanical behavior of face-centered cubic metallic ultrathin films. KEDARNATH KOLLURI, M. RAUF GUNGOR, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-3110 — We report results of large-scale molecular-dynamics simulations for the dynamic deformation under biaxial tensile strain of nanometer-scale-thick films of various face-centered cubic metals. Our results indicate that films of metals with moderate to high propensity for formation of stacking faults (e.g., Ni and Cu) exhibit an extended easy glide regime followed by a sharp increase in the material stress, whereas those with low propensity for stacking-fault formation (such as Al) exhibit a monotonic increase in the stress during dynamic loading. We find that the plastic strain rate in Cu and Ni thin films is far greater than that in Al thin films, leading to stress dissipation and an extended easy glide regime. Analysis of defect interaction mechanisms during dynamic deformation reveals dislocation annihilation, which is due to stacking-fault-mediated cross-slip mechanisms in Ni and Cu films and due to collinear interactions between dislocations in Al films.

9:48AM P23.00010 Composition dependence of the elastic constants of β and (α + βp)-phase PdHx. DOUGLAS SAFARIK, RICARDO SCHWARZ, STEPHEN PAGLIERI, DALE TUGGLE, ROBERT QUINTANA, Los Alamos National Laboratory — Previously [1], we measured the room-temperature elastic constants of PdHx for 0 < x < 0.75. These measurements were done on single crystals of α-phase Pd(H) solid solution (x < 0.01), of β-phase Pd-H hydride (x > 0.62), and of coherent two-phase mixtures of α + β phases (0.01 < x < 0.62). We found [1] that for all x the shear modulus C14 decreases linearly with x (Vegard law), whereas for 0 < x < 0.62 the shear modulus C' = (C11 + C12)/2 shows a parabolic dependence on x. We attributed [1] this unusual composition dependence of C' to thermally activated anelastic relaxations of the coherent lenticular-shaped precipitates. If this explanation is correct, then the unusual behavior of C' should disappear on cooling to low temperature. In the present work we have measured the three independent elastic constants and internal friction for both the β-phase and the coherent (α + βp)-two-phase mixture in the temperature range 1.4 < T < 296 K. We find that C14 for the (α + βp) single crystal follows a Vegard law irrespective of temperature. In contrast, C' shows deviations from the Vegard law, and these deviations grow with temperature. We discuss our results in terms of anelastic relaxations of the precipitates, and the elastic properties of two-phase composites. [1] Acta Mat. 53, 569 (2005).

10:00AM P23.00011 Adhesion Enhancement by Interfacial Microcrack Toughening. YUE QI, GM &D Center, HAIIBO GUO, University of South Carolina, XINGCHENG XIAO, GM &D Center, ZHIHUI LI, University of South Carolina — In this study, we reported a novel approach to enhance the adhesion of diamond coatings on titanium substrate by interfacial toughening. An array of oriented and confined micro-cracks around the interface was found to have the ability of opening and self-healing to release strain energy, by which to enhance macro-adhesion. Density functional theory calculations explained that cracks are energetically preferred to initiate and propagate along the (100) plane in titanium carbide interlayer. Thus by controlling the orientation of the interlayer for the failure associated with the delamination can be avoided for the coating/interlayer/substrate system.

10:12AM P23.00012 Oxide-Dispersion Strengthened Nanoparticulate Composites with Application to Magnetic Materials. ROBERT CAMMARATA, STEPHEN FARIAS, Johns Hopkins University, CHAI-LING CHIEN, Johns Hopkins University — Metal matrix nanocomposites have been fabricated by a novel electrochemical deposition method in order to produce enhanced yield strength and creep resistant materials. Metals have been synthesized from an electrolytic solution containing a suspension of oxide nanoparticles. Using a rotating disk electrode, metal samples with a uniform dispersion of oxide nanoparticles are obtained. By controlling the concentration of particles in the solution, the electrode rotation rate, and deposition current density, the volume fraction of oxide in the nanocomposite can be sensitively controlled. Low load indentation testing reveals a substantial increase in room temperature yield strength compared to single phase metals that is close to that predicted from classical hardening models. Particular attention has given to magnetic materials such as Ni and FeCo with the aim of producing materials with improved mechanical behavior without significant degradation of the magnetic properties.

10:24AM P23.00013 High pressure thermoelectricity of vanadium. DANIEL ORLIKOWSKI, LLNL — To support a larger effort for a multi-phase constitutive strength model for vanadium, we discuss the calculations performed to determine the anharmonic thermoelectricity for bcc and rhombohedral phases of vanadium. In this investigation, we have performed extensive calculations of the elastic moduli over broad ranges of temperature (<10,000 K) and pressure (<3 Mbar), accounting for both the electron-thermal and ion-thermal contributions. Using density functional theory (DFT) with the projector augmented-wave (PAW) methodology to calculate the electron-thermal component, we have combined this with the ion-thermal component, which is calculated from Monte Carlo (MC) canonical distribution averages of the strain derivatives on a multi-ion potential itself. The ion-potential is described through a many-body, quantum-based interatomic potential—the model generalized pseudopotential theory (MGPT). We suggest regions of stability for the phase diagram. The resulting elastic moduli are compared to available experimental results and to sound speeds measured along the Hugoniot.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

10:36AM P23.00014 Shock-wave dispersion and attenuation in discrete media, effect on source localization. HASSON TAVOSSI, Valdosta State University, Department of Physics, Astronomy & Geosciences, 1500 N. Patterson St. Valdosta, GA 31698 — Shock wave speed and attenuation in a non-linear discrete media are investigated. The goal of the study is to identify parameters that control shock wave or impulsive wave speed and energy dissipation in the discrete non homogeneous binary media. Material properties of solid constituents and the elastic behavior of contact points are shown to depend on the wave frequency. The behavior at both high frequency and low frequency limits are analyzed. The effects of depth on wave velocity profile, wave spectral content and attenuation are also considered. Among applications are: accurate near ground shock wave source localization by microseism waves.

Wednesday, March 18, 2009 8:00AM - 10:48AM – Session P24 DMP: Focus Session: Electron Transport in Nanotubes 326
8:00AM P24.00001 Coupling of spin and orbital motion of electrons in carbon nanotubes

Paul Mceuen, Cornell University — Electrons in atoms possess both spin and orbital degrees of freedom. In non-relativistic quantum mechanics, these are independent, resulting in large degeneracies in atomic spectra. However, relativistic effects couple the spin and orbital motion, leading to the well-known fine structure in atomic spectra. The electronic states in defect-free carbon nanotubes are widely believed to be four-fold degenerate, owing to independent spin and orbital symmetries, and also to possess electron–hole symmetry. Here we report measurements demonstrating that the spin and orbital motion of electrons are coupled, thereby breaking all of these symmetries. This spin–orbit coupling is directly observed as a splitting of the four-fold degeneracy of a single electron in ultra-clean quantum dots. The coupling favors parallel alignment of the orbital and spin magnetic moments for electrons and antiparallel alignment for holes. Our measurements are consistent with recent theories that predict the existence of spin–orbit coupling in curved graphene and describe it as a spin-dependent topological phase in nanotubes. Work done in collaboration with F. Kuemmeth, S. Ilani, and D. C. Ralph

8:36AM P24.00002 Sensitivity of carbon nanotube and graphene transistors to local atomic structure

Iddo Heller, Sohail Chatoor, Jaan Mannik, Marcel A. G. Zevenbergen, Cees Dekker, Serge G. Lemay, Delft University of Technology — Transistors based on single-walled carbon nanotubes (SWNTs) and graphene can be operated in aqueous solution where the electrolyte acts as a highly efficient gate. We show that the composition and spatial distribution of ions in the electrolyte intrinsically affect the conductance of SWNT and graphene transistors. Changes in the ionic strength, pH, and surprisingly, the type of ions affect the electronic transport through the electrostatic gating effect. In addition, changing pH leads to Schottky-barrier modification, while changing ionic strength affects the gate capacitance. Interestingly, the observed electrostatic gating effect for graphene is larger than for SWNTs. Most of our data is explained by a model that considers ionizable groups on both the underlying substrate and on the carbon surfaces. Our findings have significant implications for optimizing sensing experiments with nanocarbon transistors.

8:48AM P24.00003 Boosting electronic transport in carbon nanotubes by isotopic disorder


9:00AM P24.00004 Electrical Transport in Long Bundles of Carbon Nanotube-Metal Hybrids

Saikat Talapatra, Rakesh Shah, Clayton Schenk, Xianfeng Zhang, Department of Physics, Southern Illinois University Carbondale, Carbondale, Illinois, 62901, Swastik Kar, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180 — Although a number of works have proposed that bundles of carbon nanotubes can withstand high current densities at low resistances for high-performance applications, such structures have been demonstrated to fall short of proposed expectations. This is chiefly due to limited access to all nanotubes in a bundle in conventional two-terminal device configurations, with low number of effective conducting channels. By depositing a small quantity of high-conductance metal alloys that wet the nanotube surface, our CNT-Au/Pd alloy hybrid conductors show improved performance in terms of failure current density and resistivity. Low temperature transport measurements show that the nanotube bundles with metal coating and especially after the high-bias treatment show more and more metallic nature, with decreased negative temperature coefficient of resistance. The results will be discussed in the framework of transport theories of quasi-one dimensional systems.

9:12AM P24.00005 Phonon populations in a biased carbon nanotube transistor

Mathias Steiner, Marcus Freitag, Vasili Perebeinos, James Tsang, Joshua Small, Megumi Kinoshita, IBM T.J. Watson Research Center, Dongning Yuan, Jie Liu, Dept. of Chemistry, Duke University, Phaedon Avouris, IBM T.J. Watson Research Center — We present a comprehensive picture of the phonon populations in an electrically-driven carbon nanotube transistor, including the Raman-active G and radial breathing modes (RBM), and also the Raman-inactive zone boundary mode (K), and intermediate-frequency mode (IFP), populated by anharmonic decay. The effective temperature of the RBM is considerably lower than the intermediate- and high-frequency mode temperatures, which we explain by a phonon-decay bottleneck. We include substrate polar phonon scattering to fully account for the device electronic characteristics.


Nicola Bonini, Nicola Marzari, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Low-frequency phonon modes play an important role in the electronic and thermal transport properties of carbon nanotubes and ultrathin graphitic films. Not only they determine the very high thermal conductivity of these materials, but they also affect the electrical transport: at low bias they weakly scatter electrons, while at high bias they concur to determine the population of those optical phonon modes that most strongly limit the electrical conductivity. Quite interestingly, these low frequency phonons are also expected to couple to the vibrational modes of a surrounding material, thereby breaking all of these symmetries. This spin–orbit coupling is directly observed as a splitting of the four-fold degeneracy of a single electron in a topological phase in nanotubes. Work done in collaboration with F. Kuemmeth, S. Ilani, and D. C. Ralph

9:36AM P24.00007 Temperature-dependant current saturation in double-wall carbon nanotubes

Delphine Bouilly, Department of physics, Universite de Montreal, Canada, Matthieu Paillet, Richard Martel, Department of Chemistry, Universite de Montreal, Canada, REGROUPEMENT QUEBECOIS SUR LES MATERIAUX DE POINTE (ROMP) COLLABORATION — Current saturation is known to occur at high voltage bias in carbon nanotubes, for single-wall as well as multi-wall configurations. This saturation is generally attributed to the backscattering of carriers by optical phonons. Here we report transport measurements performed on single double-walled carbon nanotubes as a function of temperature between 77K and 400K. The good quality of the contacts between the nanotubes and the electrodes allows to observe a temperature dependence of the I-V curves. At high temperature, the saturation current shows a value around 25nA, as expected from the energy of optical phonons, but then increases non-linearly with decreasing temperature. The low-bias conductance is also measured to increase with decreasing temperature. Phenomenological models are investigated in order to explain the observed trends.

1Financial support from NSERC and FQRNT is acknowledged.
9:48AM P24.00008 Conductance Switching in Gated Graphene Nanoribbons, JESSE M. KINDER, JONATHON J. DORANDO, GARNET K.L. CHAN, Cornell University — We have investigated transport through locally gated metallic graphene nanoribbons using a numerical tight-binding method. We consider a device in which the orientation of the gate with respect to the axis of the ribbon is variable. We find that the conductance, as calculated within the nonequilibrium Green function formalism, depends strongly on the gate voltage and the orientation of the gate.

In particular, we identify specific angles at which a small change in gate voltage results in a large change in the probability of transmission. This response occurs in ribbons with zigzag or armchair edges and could provide a mechanism for a nanometer-scale electronic switch. Using the effective Dirac Hamiltonian for electrons in graphene, we provide a qualitative explanation for the ON-OFF response at particular angles and characterize its dependence on the geometry of the ribbon.

10:00AM P24.00009 Variable Range Hopping Conductivity in Carbon Nanotube Threads, CHAMINDA JAYASHINGHE, DAVID MAST, MARK SCHULZ, VESSELIN SHANOV, University of Cincinnati — We have measured the low temperature, dc electrical transport in threads spun from long multi-wall carbon nanotubes (MWCNT). The electrical transport in these threads shows variable range hopping (VRH) behavior at low temperatures, as well as non-linear IV characteristics at high applied electric fields. The MWCNT used to make the threads have an outer diameter from about 6 nm to 30 nm; these MWCNT’s have been grown in lengths up to 18 mm. The diameter of the CNT threads in this study have diameters of 15 and 25 microns; the threads were spun using 2 mm long MWCNT’s. The room temperature (RT) resistivity of the threads is on the order of 5 Ohm cm and can be changed by post-spinning treatment strategies such as high temperature annealing. From 300 K down to 4.2 K, the resistivities show an exponential dependence with temperature consistent with VRH conduction. As the RT resistivity decreases, the low temperature transport shifts from being dominated, at low temperatures, by Coulomb Gap VRH described by Efros and Shklovskii [1] to 3D-VRH as first formulated by Mott [2]. Analysis will be given of how the VRH behavior changes with intrinsic and post-treatment thread resistivity. [1] A.L. Efros and B.I. Shklovskii, J. Phys. C: Solid State Physics. 8, L49 (1975). [2] N.F. Mott, J. Non-Crist. Solids 1, 1 (1968).

10:12AM P24.00010 Experimental and computational study of 1/f noise scaling in single-walled carbon nanotube percolation films, ASHKAN BEHNAM, GIJS BOSMAN, ANT URAL, University of Florida — We study the scaling of 1/f noise in single-walled carbon nanotube percolation films as a function of device parameters and film resistivity both experimentally and computationally. Our experiments were performed on single-walled carbon nanotube arrays grown on indium tin oxide (ITO) substrates. The nanotube length distribution was characterized by a mean length of 20 μm and a standard deviation of 10 μm. The geometrical characteristics of these nanotube arrays were captured by scanning electron microscopy (SEM). We measured the 1/f noise in several p-n junctions in the percolation regime at room temperature using current fluctuations at 100 mV applied bias. We also computed the 1/f noise in this regime using a percolation theory framework. In this study, we measured the magnitude of the 1/f noise and its scaling exponent for a range of device parameters such as area, thickness, and resistivity. We observed a scaling exponent of approximately 1.2 for a large range of resistivities and found that the noise amplitude depends strongly on device dimensions, nanotube degree of alignment, and the film resistivity, following a power-law relationship with resistivity near the percolation threshold after properly removing the effect of device dimensions. We also find that the critical exponents associated with the noise-resistivity and noise-device dimension relationships are not universal invariants, but rather depend on the specific parameter that causes the change in the resistivity and 1/f noise, and the value of the other device parameters. Since 1/f noise is a more sensitive measure of percolation than resistivity, these results not only provide important fundamental physical insights into the complex interdependencies associated with percolation transport in nanotube films, but also help understand and improve the performance of these nanomaterials in potential device applications, such as nanoscale sensors, where noise is an important figure of merit.

10:24AM P24.00011 Anisotropic Terahertz Response of Highly Aligned Single-Walled Carbon Nanotubes, L. REN, X. WANG, L. BOOSHEHRI, D. HILTON, J. KONO, I. KAWAYAMA, M. TONOUCHI, Inst. of Laser Eng., Osaka University — Dynamic conductivities of degenerate 1-D electrons are expected to provide a wealth of information on quantum confinement, electron interactions, and disorder. Here, we use terahertz time-domain spectroscopy (THz-TDS) to determine the complex dielectric function of a thin film of highly aligned single-walled carbon nanotubes (SWNTs) on sapphire. The THz electromagnetic wave used was linearly polarized, and the measured dielectric function was very anisotropic. As the angle between the nanotube axis and the THz electric field changed, anisotropy was clearly observed for both the real and imaginary parts of the dielectric function. The absorption of the THz wave decreased monotonically with increasing angle from 0 to 90 degrees, with maximum and minimum absorption at 0 and 90 degrees, respectively. Through a proper model, the complex dynamic conductivity was extracted and showed a non-Drude-like frequency dependence, with the real part increasing monotonically with increasing frequency between 0.2 and 1.8 THz.

10:36AM P24.00012 Carbon nanotube diode performance and photovoltaic response, DANER ABDULA, MOONSUB SHIM, University of Illinois Urbana-Champaign — Due to their unique electronic properties, carbon nanotubes have been at the forefront in the development of next generation electronic devices. The p-n diode is arguably the most pivotal electronic and photovoltaic device. Up to now, nanotube diodes have had significant drawbacks including complex quad-terminal device geometries to achieve electrostatic doping, large series resistances from the inclusion of an intrinsic region at the junction, unstable n-type doping, and Zener breakdown. We have developed a method to create two terminal abrupt junction diodes from single semiconducting carbon nanotubes with simple photo-patterned polymer layers defining air-stable p- and n-regions. These intratube diodes show nearly ideal behavior with relatively low series resistance and no sign of Zener breakdown at room temperature. Spatial doping profiles measured by micro-Raman spectroscopy and selective electrochemical gating of the n-region indicate that diode performance depends strongly on relative doping levels. A short circuit current of 1.4 nA with an open circuit voltage of 205 mV are measured when illuminated to saturation.

Wednesday, March 18, 2009 8:00AM — 11:00AM Session P25 DMP: Focus Session: Graphene VII: Electronic Properties

8:00AM P25.00001 Cyclotron Resonance at the Dirac Point, PAUL CADDEN-ZIMANSKY, Columbia University/NHMF, ERIK HENRIKSEN, Columbia University, ZHIGANG JIANG, Georgia Tech University, LI-CHUN TUNG, NHMF, MOLLIE SCHWARTZ, Columbia University, YONG-JIE WANG, NHMF, PHILIP KIM, Columbia University, HORST STORMER, Columbia University/Bell Labs — We present high field infrared spectroscopy data on the n = -1 and n = 0 graphene quantum dots. Our results indicate that the bare Zeeman splitting naively expected for a spin-split state. We compare the field dependence of the shifts with proposed degeneracy-breaking mechanisms.

8:12AM P25.00002 Hydrodynamic approach to transport in graphene, RAFI BISTRITZER, ALLAN MACDONALD, University of Texas at Austin — Exploiting the strong electron-electron interactions in graphene we construct a hydrodynamic theory in which the carrier dynamics is described by three parameters: the electronic temperature, the chemical potential and the drift velocity. We use this theory to describe both linear and non linear transport in graphene.

9:00AM P25.00004 Energy Relaxation of Hot Dirac Fermions in Graphene1, WANG-KONG TSE, University of Texas, Austin; University of Maryland, College Park, SANKAR DAS SARMA, University of Maryland, College Park — We develop a theory for the energy relaxation of hot Dirac fermions in graphene. We obtain a generic expression for the energy relaxation rate of hot Dirac fermions in graphene due to electron-phonon interaction and calculate the power loss due to both optical and acoustic phonon emission as a function of electron temperature $T_e$ and density $n$. We find an intrinsic power loss weakly dependent on carrier density and non-vanishing at $n = 0$, originating from interband electron-optical phonon scattering from the intrinsic electrons in the Dirac valence band. We also obtain the total power loss per carrier to be $\sim 10^{-12}$ and $10^{-11}$ for within the range of electron temperatures $\sim 20 - 1000 K$, finding that the temperature for the optical phonon emission to overtake acoustic phonon emission as the dominant energy loss mechanism ranges $\sim 200 - 300 K$ for $n = 10^{11} - 10^{13} cm^{-2}$.

1This work is supported by US-ONR, NSF-NRI, and SWAN SRC.

9:12AM P25.00005 Electron and hole puddles in monolayer graphene on SiO$_2$, B.J. LEROY, A. DESHPANDE, University of Arizona, W. BAO, F. MIAO, C.N. LAU, University of California at Riverside — We have performed spatially resolved scanning tunneling spectroscopy measurements on single layer graphene. The graphene was prepared on SiO$_2$ by the mechanical exfoliation technique and an electrode was attached by electron beam lithography. Atomically resolved topography images over 40 nm areas show that the graphene conforms to the SiO$_2$ surface as well as having intrinsic ripples. In addition to the topography measurements, we have mapped the local density of states as a function of position and energy. We observe a spatially varying Dirac point which leads to electron and hole puddles at low energy. These puddles have a characteristic size scale of about 5 nm. The puddles arise due to curvature in the graphene film which induces shifts in the chemical potential as well as long range scattering from charged impurities.

9:24AM P25.00006 Ripples on graphene and their effect on lattice and electronic properties, MIKHAIL KATSNELSON, Radboud University Nijmegen — A discovery of graphene, a new allotrope of carbon [1], representing the simplest, one-atom thick, membrane, opens exciting perspectives in statistical physics of two-dimensional systems in general. As expected from theory of flexible membranes [2], free suspended graphene is corrugated (rippled) due to thermal bending fluctuations, which was confirmed by experiment [3] and atomistic simulations [4]. This makes graphene strongly anharmonic crystal leading to anomalous temperature dependences of its thermal expansion, elastic moduli and other thermodynamic and mechanical properties. The ripples are also a source of pseudomagnetic gauge field [5] acting on Dirac fermions which leads to important consequences for the electronic structure such as a formation of midgap states [6,7]. Quenched ripples can be also important sources of electron scattering limiting charge-carrier mobility in graphene [8]. Possible mechanisms of this quenching are discussed.


10:00AM P25.00007 Rippling of Graphene1, MARIA MOURA, UT Austin Physics Department, REbecca THOMPson-FLAGG, APS PhysicsCentral, MICHAEL MARDER, UT Austin Physics Department — Experiments found that free standing single-layer graphene sheets display ripples (see ref. Meyer et al. Nature 446, 60 2007). Here we show that these ripples can be a consequence of adsorbed molecules sitting on random sites. The adsorbates cause the bonds between the carbon atom to lengthen slightly. Static buckles caused by roughly 20 % coverage of adsorbates are consistent with experimental observations. We explain why this mechanism is more likely to explain ripples than are thermal fluctuations or the Mermin-Wagner theorem (previously invoked).

1National Science Foundation DMR 0701373.

10:12AM P25.00008 Spectroscopy and Reflection Properties of Massive Graphene[1], KEVIN KNOX, MEHMET YILMAZ, Columbia University, SHANCAI WANG, Renmin University of China, ALBERTO MORGANTE, University of Padua, DEAN Cvetko, University of Ljubljana, ANDREAS KLOSE, TU Berlin, ANDREAS LOOS, University of Munich, MARIA MOURA, UT Austin Physics Department, REBECCA THOMPSON-FLAGG, APS PhysicsCentral, MICHAEL MARDER, UT Austin Physics Department — We develop a theory for the energy relaxation of massive Dirac fermions due to phonon scattering in graphene. We obtain an analytic expression for the energy relaxation rate of massive Dirac fermions in graphene due to electron-phonon interaction and calculate the power loss as a function of electron temperature $T_e$ and density $n$. We find that the energy relaxation rate is weakly dependent on carrier density and non-vanishing at $n = 0$, originating from interband electron-optical phonon scattering from the intrinsic electrons in the Dirac valence band. We also obtain the total power loss per carrier to be $\sim 10^{-12}$ and $10^{-11}$ within the range of electron temperatures $\sim 20 - 1000 K$, finding that the temperature for the optical phonon emission to overtake acoustic phonon emission as the dominant energy loss mechanism ranges $\sim 200 - 300 K$ for $n = 10^{11} - 10^{13} cm^{-2}$.

10:24AM P25.00009 Kohn-Luttinger superconductivity in graphene, JOSE GONZALEZ, Universidad de de la Materia, CSIC, Madrid (Spain) — We address the development of superconductivity in graphene when the Fermi level becomes close to one of the Van Hove singularities of the electron spectrum. The different segments of the Fermi line show then an approximate nesting, which enhances unconventional superconducting and magnetic correlations for a dominant repulsive interaction. The origin of the pairing instability lies in the strong anisotropy of the e-e scattering along the Fermi line, leading to a channel with attractive coupling when making the projection of the BCS vertex on the symmetry modes with nontrivial angular dependence. We show that the superconducting instability is particularly strong at the Van Hove singularity in the valence band of graphene, where the critical scale may be pushed up to temperatures larger than 1 K, depending on the ability to tune the Fermi level to the proximity of the singularity.

10:36AM P25.00010 Polarization and Spectral Properties of Massive Graphene, VALERI KOTOV, VITOR PEREIRA, Boston University, BRUNO UCHOA, Boston University and UIUC, ANTONIO CASTRO NETO, Boston University — We discuss the situation when a finite gap exists in the Dirac fermion spectrum, due to either external factors (substrate-induced), or the mesoscopic (finite size) nature of the sample. The gap could also be generated dynamically via chiral symmetry breaking. We will overview: (1.) The behavior of the polarization charge, induced by an external Coulomb source. The charge density exhibits an unconventional distribution is space, which we present in detail. The density variation could be observable in real experiments when an external ion is placed on the graphene sheet. (2.) The modification of the fermion self-energy, in particular, the large-$N$ limit of the theory. We find that in this limit, which could be relevant for Graphene, the electronic dispersion is strongly renormalized at small energies. We discuss possible consequences of this behavior.
10:48AM P25.00011 High-Mobility Dual-gated Graphene Field-Effect Transistors with Al2O3,Dielectric1 SEYOUNG KIM, JUNCHYO NAH, INSUN JO, DAVID SHAHRIRDI, The University of Texas at Austin, LUIGI COLOMBO, Texas Instruments, ZHEN YAO, EMANUEL TUTUC, SANJAY BANERJEE, The University of Texas at Austin — The carrier mobility in graphene field-effect transistors (GFETs) is primarily dominated by the extrinsic impurity scattering, such as charged impurities in the dielectric. Therefore, the impact of a top-gate dielectric stack on the transport characteristics of graphene represents a key issue for high-performance GFETs. Here, we present the fabrication and characterization of dual-gated graphene FETs and dual-gated graphene devices with Hall bar geometry using Al2O3 as top-gate dielectric. We use a thin Al film as a nucleation layer to enable the atomic layer deposition of Al2O3. Our FETs show mobility values of over 6,000 cm2/Vs at room temperature, a finding which indicates that the top-gate stack does not significantly increase the carrier scattering, and consequently degrade the device characteristics. We propose a device model to fit the experimental data with a single mobility value.

1This work was supported by SWAN-NRI, DARPA and NSF.

Wednesday, March 18, 2009 8:00AM - 11:00AM
Session P26 DMP: Focus Session: Graphene VIII: Electronic Properties 328

8:00AM P26.00001 Experimental studies of the transport in graphene in a parallel magnetic field at low temperatures1 LIUYAN ZHANG, JORGE CAMACHO, Brookhaven National Laboratory, HELIN CAO, ISAAC CHILDRES, YONG CHEN, Purdue University, ALEXEI TSVELIK, DMITRI KHARZEEV, MAXIM KHODAS, MYRON STRONGIN, TONICA VALLA, IGOR ZALIZNYAK, Brookhaven National Laboratory, BROOKHAVEN NATIONAL LABORATORY COLLABORATION, PURDUE UNIVERSITY COLLABORATION — Graphene has remarkable electronic properties, and it is also a very promising material for spintronic applications. Most previous experiments, however, were focused on studying graphene devices in perpendicular magnetic field, which quantizes the real-space motion of Dirac electrons in graphene and leads to an unusual quantum Hall effect. Here we present the results of experimental studies of electric transport in single- and few-layer graphene devices in parallel magnetic field and at low temperatures. The Dirac-point resistance of our graphene devices was studied as a function of magnetic field and temperature. The effect of tuning the chemical potential under different magnetic fields was also investigated and will be discussed.

1This work was supported by the US Department of Energy, and Purdue University.

8:12AM P26.00002 The Image Potential for Graphene with an Electrostatic Grating1 GODFREY GUMBS, Hunter College/CUNY, DANHONG HUANG, USAF Research Lab, PEDRO ECHENIQUE, DIPC, Donastia, San Sebastian — We calculate the surface response function and the image potential of a layered structure of two-dimensional (2D) electron systems (ES). A point charge is placed at a distance away from the surface which is in the xy-plane. These 2D layers are coupled through the Coulomb interaction and there is no interlayer electron hopping. The separation between adjacent layers can be adjusted to investigate the role which layer separation and the number of layers play on both the surface response function and the image potential. Specifically, we consider the system composed of graphene layers or the layered 2D electron gas (EG) formed at the interface of a semiconductor heterostructure such as GaAs/AlGaAs. We show that the image potential for graphene is qualitatively the same as for the 2DEG. We examine the way in which the image potential is modified by applying a one-dimensional periodic electrostatic potential (through a gated grating for modulation). These results indicate that the charge screening for graphene is not much different from the 2DEG.

1Supported by contract FA 9535-07-C-0207 of AFRL.

8:24AM P26.00003 Adsorption of Ammonia on Graphene1 PRASOON JOSHI, Electrical Engineering Department, Pennsylvania State University, HUGO ROMERO, AWNIL GUPTA, HUMBERTO GUTIERREZ, MILTON COLE, Physics Department, Pennsylvania State University, SRINIVAS TADIGADAPA, Electrical Engineering Department, Pennsylvania State University, PETER EKLUND, Physics Department, Material Science & Engineering Department — We report on experimental studies of NH3 adsorption/desorption kinetics on graphene surfaces. The study employs bottom-gated graphene field effect transistors (FETs) supported on Si/SiO2 substrates. Detection of NH3 occurs through the shift of the source-drain resistance maximum (“Dirac peak”) with gate voltage. The observed shift of the Dirac peak toward negative gate voltages in response to NH3 exposure is attributed to the charge transfer from adsorbed NH3, with the amount of charge estimated to be ∼0.06 electrons per molecule. The sorption kinetics of our FET devices is well described by the sum of two exponential terms corresponding to a fast and a much slower process, whose time constants differ by a factor of ∼9. The two-time constant sorption kinetics is consistent with Fickian-type diffusion of NH3 from the interstitial pockets formed at the interface between the graphene and the supporting SiO2 gate dielectric.

1NSF NIRT # ECS 06-09243

8:36AM P26.00004 Resistive-free method for contacting graphene and few-layer graphene CATERINA SOLDANO, CEMES - Centre d Elaboration de Mateiaux et d Etudes Structurales Toulouse, France, JORGE CAMACHO, Brookhaven National Laboratory, HELIN CAO, ISAAC CHILDRES, JEREMIE GRISOLIA, Department of Genie Physique, INSA, Toulouse, France — We report on experimental studies of NH3 adsorption/desorption kinetics on graphene surfaces. The study employs bottom-gated graphene field effect transistors (FETs) supported on Si/SiO2 substrates. Detection of NH3 occurs through the shift of the source-drain resistance maximum (“Dirac peak”) with gate voltage. The observed shift of the Dirac peak toward negative gate voltages in response to NH3 exposure is attributed to the charge transfer from adsorbed NH3, with the amount of charge estimated to be ∼0.06 electrons per molecule. The sorption kinetics of our FET devices is well described by the sum of two exponential terms corresponding to a fast and a much slower process, whose time constants differ by a factor of ∼9. The two-time constant sorption kinetics is consistent with Fickian-type diffusion of NH3 from the interstitial pockets formed at the interface between the graphene and the supporting SiO2 gate dielectric.

8:48AM P26.00005 Transport studies of highly oriented pyrolytic graphite ARUNA N. RAMANAYAKA, BHASKAR KAVIRAJ, RAMESH G. MANI, Department of Physics & Astronomy, Georgia State University — Highly Oriented Pyrolytic Graphite (HOPG) consists of stacked sheets of single layers of carbon with weak interlayer interactions, which gives rise to anisotropic transport with striking differences between in-plane and perpendicular transport. Transport studies of single layers of carbon, known as Graphene, have shown striking new features in two dimensional transport, arising from the linear dispersion relation and analogies to quantum electrodynamics. A question of interest for our experiments is to examine the crossover from Graphite to Graphene and trace the three-dimensional to two-dimensional evolution in the transport properties of the layered carbon system. Hence, we report here on our efforts to fabricate specimens starting from commercially available HOPG, and present measurements in magnetic fields up to 12 Tesla, down to 1.5 K.

9:00AM P26.00006 ABSTRACT WITHDRAWN
9:12AM P26.00007 Semiclassical model for the magnetoresistance and Hall coefficient of inhomogeneous graphene$^1$, RAKESH TIWARI, DAVID STROUD, The Ohio State University — We show that when bulk graphene breaks into n-type and p-type puddles, the in-plane resistivity becomes strongly field dependent in the presence of a perpendicular magnetic field, even if homogeneous graphene has a field-independent resistivity. We calculate the longitudinal resistivity $\rho_{xx}$ and Hall resistivity $\rho_{xy}$ as a function of field for such a system, using the effective-medium approximation. The conductivity tensors of the individual puddles are calculated using a standard Boltzmann approach suitable for the band structure of graphene near the Dirac points. The resulting resistivity saturates, provided that the area fractions $f_n$ and $1 - f_p$ of n and p type puddles are slightly unequal, and agrees with experiments if the relaxation time is weakly field-dependent. The Hall resistivity $\rho_{xy}$ found to change sign at $f_n = 1/2$.

3Work supported by the Center of Emergent Materials at the Ohio State University through NSF MRSEC (DMR-0820414)

9:24AM P26.00008 Anomalous Quantum Oscillations in Graphene Hybrid Structures, CONOR PULS, NEAL STALEY, YING LIU, The Pennsylvania State University, Department of Physics — It is well recognized that the edge states of graphene are interesting and important for both fundamental inquiry and potential practical applications of graphene. However, states associated with a step found in a continuous sheet of graphene with two different thicknesses have not been explored to date. We report a study of graphene hybrid structures featuring such a step. In a bulk hybrid featuring two large-area one- and two-layer graphene, two sets of Landau levels and features related to the interface were found. In edge hybrids featuring a large two-layer graphene with narrow one-layer graphene edges, we observed an anomalous suppression in quantum oscillation amplitude due to the locking of one- and two-layer graphene Fermi energies by charge transfer across the interface. These findings demonstrate the existence of unique interface states and related phenomena deserving of further studies. We will also report relevant studies on epitaxially-grown graphene films.

9:36AM P26.00009 Graphene mediated exchange bias$^1$, YURIY SEMENOV, JOHN ZAVADA, KI WOOK KIM, NCSU, DEPARTMENT OF ECE TEAM — We have theoretically investigated the role of graphene in mediating the indirect exchange interaction when it is placed between two ferromagnetic dielectric materials. The calculation based on a tight-binding model illustrates that the magnetic interactions at the interfaces affect not only the graphene band structure but also the thermodynamic potential of the system. This induces an indirect exchange interaction between the magnetic layers that can be considered in terms of an effective exchange bias field. The analysis clearly indicates a strong dependence of the effective exchange bias on the properties of the mediating layer. Through the dependence on the graphene electro-chemical potential, the effective exchange bias can be modulated electrically over a wide range even at room temperature. This dependence also results in qualitatively different characteristics for the cases involving monolayer and bilayer graphene. The numerical estimate indicates the potential significance of the proposed phenomenon in practical applications.

This work was supported in part by the DARPA and the FENA

9:48AM P26.00010 Conductivity engineering of graphene by defect formation, BIPLAB SANYAL, Uppsala University — Graphene exhibits exotic electronic properties revealed in transport measurements. The possibility to influence the electronic structure and hence control the conductivity by physisorption or doping with adatoms is crucial in view of electronics applications. Here we show that in contrast to expectation, the conductivity of graphene increases with increasing concentration of vacancy defects, with an amount of over one order of magnitude. We obtain a pronounced enhancement of the conductivity after insertion of defects by ab-initio electronic structure calculations. The theoretical results are supported by the experimental studies on carbon nano-sheets. Our finding is attributed to defect induced mid-gap states, which create a region exhibiting metallic behavior around the vacancy defects. The modification of the conductivity of graphene by implementation of stable defects is crucial for the creation of electronic junctions in graphene-based electronics.

10:00AM P26.00011 A computational study of electrical transport in graphene-based films and composites, JEREMY HICKS, ASHKAN BEHNAM, ANT URAL, Electrical and Computer Engineering, University of Florida — We study the electrical behavior of films and composites composed of a mesh of graphene sheets using Monte Carlo simulations. We take into account the sheet-sheet junctions with different areas as well individual graphene sheets in calculating the film/composite transport properties. We find that the resistivity of composites varies by many more orders of magnitude than films approaching the percolation threshold due to tunneling-percolation through the sheet network, but otherwise the two exhibit many of the same scaling trends. Furthermore, we find that resistivity in both cases is a strong function of graphene sheet aspect ratio, density, volume fraction, and device dimensions. We extract important parameters such as the critical exponents near the percolation threshold and compare them with the available experimental data. These results, explained through physical and geometrical arguments, give valuable insights into the factors influencing the electrical transport in graphene sheet films and nanocomposites. Such graphene-based nanomaterials might find applications in many fields such as photovoltaics, sensors, and multifunctional nanocomposites.

10:12AM P26.00012 Investigating the quantum behavior of a graphene-based Josephson Junction, JOSEPH LAMBERT, ZECHARIAH THRALLKILL, ROBERTO RAMOS, Drexel University — Recent experiments have demonstrated the Josephson effect in superconducting mesoscopic graphene devices consisting of two superconducting leads separated by a few hundred nanometers, contacted by single and multiple layers of graphene [1]. We report on the progress of low temperature experiments that study the temperature dependence of switching currents in this device. The motivation is to explore the presence of macroscopic quantum metastable states similar to those found in current-biased Josephson junctions. These states are interesting and have been used as basis states for superconducting qubits. [1] H.B. Heersche, P.D. Jarillo-Herrero, J.B. Oostinga, L.M.K. Vandersypen, and A.F. Morpurgo, Induced superconductivity in graphene, Solid state communications, 143(1-2), 72-76 (2007)

10:24AM P26.00013 Study on the Electronic Band Structures of Doped Graphene, C.G. HWANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, KEVIN T. CHAN, D. SIEGEL, Department of Physics, University of California, Berkeley, CA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, A.V. FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, MARVIN L. COHEN, Department of Physics, University of California, Berkeley, CA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, J.B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, A. LANZARA, Department of Physics, University of California, Berkeley, CA, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA — A carbon sheet self-assembled on a SiC substrate, has been found to undergo changes in an electronic property as a function of doping concentration. Depending on the species of dopants, charge carrier density is gradually modified with increasing dopant coverage. By using angle resolved photoemission spectroscopy, we study how the graphene pi bands are modified by changing doping concentration and we discuss the effect of doping on many-body interaction such as electron-phonon coupling. These results provide new information on the role of electron-phonon coupling for superconductivity in the graphite intercalated compounds.
10:36AM P26.00014 Anomalous thermoelectric transport of Dirac particles in graphene. PENG WEI, WENZHONG BAO, YONG PU, CHUN NING (JEANIE) LAI, JING SHI, Department of Physics, University of California at Riverside — We report a thermoelectric transport property study of single layer graphene devices in both classical and quantum Hall regimes. In zero magnetic field, by sweeping the gate voltage $V_g$ to vary the carrier density $n_{2D}$, we demonstrate a diverging behavior in the Seebeck coefficient $S_{xx}$, i.e. $S_{xx} \sim 1/\sqrt{n_{2D}}$, which is a direct consequence of the linear energy dispersion of the massless particles. At low temperatures and high carrier densities, the Seebeck coefficient depends linearly on temperature, indicating the validity of the Mott relation. In the applied magnetic fields, we observe an anomalously large Nernst signal ($\sim 6 \mu V/K\mu T$) at the Dirac point. This is another unusual property expected for massless particles. At low temperatures where the quantum Hall effect is observed, both the Seebeck and Nernst signals show oscillations corresponding to the Landau levels manifested in the quantum Hall plateaus.


Wednesday, March 18, 2009 8:00AM - 11:00AM
Session P27 GIMS: Focus Session: Advances in Scanned Probe Microscopy III: High Frequency and Optical Techniques 329

8:00AM P27.00001 Nanoscale Spectroscopy with Optical Antennas, LUKAS NOVOTNY, University of Rochester — Antennas are devices that efficiently convert localized energy to free propagating radiation, and vice versa. They are a key enabling technology in the microwave and radio-wave regime but their optical analogue is greatly unexplored. In order to understand antenna-coupled light emission and absorption we use a single molecule as an elementary light emitting device. With an optical antenna in the form of a simple gold particle we are able to increase the emission efficiency by more than a factor of 10. However, for very short distances between particle and molecule the fluorescence yield drops drastically because of nonradiative energy transfer. A simple gold particle is not an efficient optical antenna and it can be expected that favorably designed nanoplasmic structures will yield much higher enhancement. Optical antennas can be employed as light sources for high-resolution optical microscopy and spectroscopy. We demonstrate vibrational (Raman scattering) and nonlinear imaging with spatial resolutions down to 10nm.

8:36AM P27.00002 Nano-Prism Probe for Nano-Optical Applications, TAEKYEONG KIM, BYUNG YANG LEE, SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University, DEOK-SOO KIM, ZEE HWAN KIM, Department of Chemistry, Korea University — Recently, a nano-prism structure has drawn attention as an optical nano-antenna due to its exotic optical properties, while it has been extremely difficult to prepare a probe terminated with a nano-prism for nano-optical applications. Herein, we report a method to mass-produce pristine nano-prism probes. Our fabrication process resulted in nano-prism with sharp edge at the end of the probe, which significantly enhanced the electric field around it and made nano-prism probes ideal for nano-optical applications. We performed the apertureless near-field scanning optical microscopy on gold nanoparticles using a nano-prism probe, revealing the field localization at the vertices of the nano-prism. We also demonstrated the fabrication of multiple nano-prism probes in a parallel fashion. This method could be a major breakthrough and provide tremendous flexibility for SPM optical applications such as nano-TERS (tip enhanced Raman scattering) or FRET (fluorescent resonance energy transfer) because it allows one to mass-produce nano-probes terminated virtually general nanostructures. (Advanced Materials, in press)

8:48AM P27.00003 Optical Response of Absorbates in the STM Environment; The Influence of the STM Tip and Plasmonic Effects, PING CHU, D.L. MILLS, University of California, Irvine — STM is widely used to explore the excited states and related optical properties of adsorbates on metal surfaces. The adsorbate may be placed on a thin oxide layer that is grown on the metallic substrate. One may ignore the direct hybridization between the adsorbate electrons and those in the substrate. We have developed the theory of the optical response of adsorbates in such an environment. Electrons in the adsorbate may interact with the electronic degrees of freedom of the tip/substrate complex through the fluctuating electric fields generated by the zero point motions of electrons in the substrate and the tip. The coupled plasmons of the tip/substrate complex contribute to these fluctuating fields. We have developed a formalism which allows us to describe energy level shifts of the adsorbate orbitals and the non radiative decay rate of excited states from coupling to the electronic degrees of freedom in the tip and substrate. We have also developed a theory of plasmon enhanced radiation emission under the tip, where the coupled plasmons of the tip/substrate complex are responsible for the enhancement of the emission.

1Research supported by the U. S. DOE, Grant No. DE-FG03-84ER-45083.

9:00AM P27.00004 Ultrafast Stroboscopic Optical Interferometry of Nanoelectromechanical Devices in Damping Pressurized Gas Environment, O. SVITSELSKIY, V. SAUER, N. LIU, K.M. CHENG, M.R. FREEMAN, W.K. HIEBERT, University of Alberta Physics Dept and National Institute for Nanotechnology, Edmonton AB Canada — A broad range of prospective applications of nanoelectromechanical devices necessitates understanding their performance under varying external conditions. We report a comprehensive gas damping study of a series of Si nanoribbons and nanocantilevers with thickness of 0.147 µm, widths ranging from 0.1 to 1 µm, and lengths from 0.5 to 12 µm. Free ring-down oscillations of the resonators, capacitively excited by 1 ns 50 V electric pulses, were measured via instantaneous optical interference pictures snapped by a femtosecond laser. The decay response to a range of damping environments was studied, including response to different gases (He, N₂, CO₂) in widely ranging pressures from deep vacuum up to 200 bar, all done in a specially designed scanning optical microscopy chamber [1]. The resonator parameters demonstrate three distinct regions of pressure behavior: high vacuum, free molecular flow, and viscous. For each region a qualitative model is presented. [1] O.Svitsel'skiy et al, Rev.Sci.Instr.79 093701, 2008

9:12AM P27.00005 An Ultra High Vacuum Radio Frequency Scanning Tunneling Microscope, UTKU KEMIKTARAK, Dept. of Physics, Boston University, Boston, MA 02215, KEITH SCHWAB, Dept. of Physics, Cornell University, Ithaca NY 14853, KAMIL EKINCI, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 and Dept. of Mechanical Eng., Boston University, Boston, MA 02215 — Radio frequency scanning tunneling microscope (RF-STM) utilizes a LC resonant circuit to achieve impedance matching between the STM tunnel junction and 50-Ω high frequency electronics. This technique allows measurement bandwidths up to 10 MHz. We have built an ultra high vacuum (UHV) RF-STM system with in-situ tip and surface treatment as well as sample, tip and matching circuit exchange. In this talk, we will describe the basic operation of this system and discuss the application of UHV RF-STM to high frequency displacement detection. We will argue that UHV RF-STM is a suitable tool to measure back-action forces of tunneling electrons and other tip-sample interactions.
9:24AM P27.00006 Development of a scanning probe microscope for localized ferromagnetic resonance measurements. CHRISTIAN LONG, NAOYUKI TAKETOSHI, University of Maryland, HAITAO YANG, Intumatic Corporation, ICHIRO TAKEUCHI, University of Maryland — We present an update on our research into the development of a scanning probe microscope capable of performing localized ferromagnetic resonance measurements. The system is based on near-field microwave microscopy using a resonant microwave cavity. Using near-field microwave microscopy allows us to produce a GHz frequency magnetic field which is confined to the region around the probe tip. By recording the change in the transmission coefficient of the resonator (S12) as a function of applied DC magnetic field, we measure the absorption of RF energy by the sample. The resulting ferromagnetic resonance spectrum allows us to map the magnetic properties of the material under the probe tip. The possibility to perform localized ferromagnetic resonance measurements using a scanning probe geometry promises to yield new insight into the properties of magnetic thin films.

9:36AM P27.00007 Scanning magnetic resonance microscopy: Spatially resolved imaging of ferromagnetic resonance on yttrium iron garnet disk. TOSHU AN1, TOYOAKI EGUCHI, YUKIO HASEGAWA, The Institute for Solid State Physics, The University of Tokyo — We developed a radio frequency (RF) probe which can be implemented into scanning probe microscopy aiming for its spatially resolved imaging. The probe is composed of a sharp tip attached at the end of a semi-rigid coaxial cable which transmits RF over 10 GHz. To measure ferromagnetic resonance (FMR) of a sample, the probe is set close to the sample, and the S11 parameter was measured by using a network analyzer. As a test magnetic sample, a 10 mm-diameter and 1 mm-thickness polycrystalline YIG (yttrium iron garnet) disk was used. By locating the RF probe at the center of the YIG disk, FMR signal was detected as an absorption dip at 2.8 GHz in the S11 measurements under in-plane static magnetic field of 458 Oe. The detected FMR signal has a sharper dip compared with that obtained in the coplanar wave guide method, and by moving the RF probe to the edge of the YIG disk, two different frequencies of FMR signal appears depending on the moving direction parallel or perpendicular to the applied magnetic field. The detected spatially dependent FMR signals are well explained by the magnetostatic waves.

1PRESTO, Japan Science and Technology Agency

9:48AM P27.00008 Design and Fabrication of a Nanoscale Force Sensor for High-Speed Atomic Force Microscopy. J. M. CAMPBELL, B. LUCHT, R. G. KNOBEL, Queens University — The atomic force microscope (AFM) has become an important tool in many fields ranging from materials science to biology. Conventional microfabricated AFM cantilevers have resonance frequencies of 10–300 kHz; some specialized cantilevers are available with frequencies up to 2 MHz. However, this represents the practical limit of the resonance frequency of microcantilevers. Three modeling methods were used to design a 200 MHz silicon nitride cantilever suitable for integration into an atomic resolution, frequency-modulation AFM. A process was developed to fabricate the cantilever coupled to an atomic point contact (APC) displacement detector, a device first demonstrated by Flowers-Jacobs et al. (2007). The cantilever mask and APC electrodes were defined through electron-beam lithography and triple-angle evaporation. The cantilever pattern was transferred to the nitride layer through focused ion beam milling and a subsequent wet etch into the underlying Si substrate suspended the structure. Then, using an active feedback system similar to that developed by Strachan et al. (2005), electromigration was used to form the APC at 77 K and 10−6 Torr. Progress toward measuring cantilever motion with the APC displacement detector through microwave reflectometry will be discussed.

10:00AM P27.00009 Interferometric and Synthetic Aperture Real-Time Terahertz Imaging 1. KE SU, ZHINWEI LII, DAME E. GARY, JOHN F. FEDERICI, Department of Physics, New Jersey Institute of Technology, ROBERT B. BARAT, Otto York Department of Chemical Engineering, New Jersey Institute of Technology, ZOI-HELENI MICHALOPOULOUL, Department of Mathematical Sciences, New Jersey Institute of Technology — Over the past several years, several methods of real-time THz imaging have been developed. In this presentation, we describe a synthetic aperture imaging method of THz imaging. A 4-element THz detector array is used to reconstruct 2-D images of a point source through the interferometric synthetic aperture imaging method. A capture rate up to 63 frames/s can be achieved. The recorded video showing the movement of the terahertz source in real time can be viewed at http://www.njit.edu/~ks265/imagingvideo.html after baseline and phase correction. Furthermore, a high power THz source will be integrated in this CW THz system for longer stand-off imaging distances.

1This work is supported by US Army, Picatinny Arsenal

10:12AM P27.00010 Fabrication of MEMS Bimaterial Sensors for Uncooled THz Imaging. DRAGOSLAV GROBOVIC, GAMANI KARUNASIRI, Naval Postgraduate School — Recently, there has been a significant interest in Terahertz (THz) technology, primarily its applications in concealed object detection and medical imaging. THz region of the spectrum has been underutilized due to lack of compact and efficient sources and detectors. THz imaging has recently been achieved using uncooled, microbolometer infrared (IR) camera and quantum cascade laser (QCL) operating as a THz illuminator. However, bolometer IR cameras are not optimized for the THz band and fabrication of their focal plane arrays (FPAs) is complex due to required monolithic integration of detectors and readout electronics. Recent developments in bi-material based IR FPAs with optical readout, substantially simplify the fabrication process by decoupling readout from sensing. This presentation describes the design and fabrication of THz-optimized bi-material FPAs, as well as integration of the real-time imaging system. The detection scheme involves detector deformation to minute temperature changes due to absorption of THz radiation. Individual detector deformations are simultaneously probed by shining visible light on entire FPA and reflecting it into a CCD camera. Optical readout eliminates the self-heating effects, enabling longer integration times and, better signal-to-noise ratio.

1This work is supported by the AFOSR

10:24AM P27.00011 Detection of terahertz radiation from 410 GHz CMOS circuit and other high-frequency oscillators using a Fourier Transform Interferometer 1. EUNYOUNG SEOK2. Department of Electrical and Computer Engineering, University of Florida, DANIEL J. ARENAS, Department of Physics, University of Florida, DONGHA SHIM, KENNETH K. O, Department of Electrical and Computer Engineering, University of Florida, DAVID B. TANNER, Department of Physics, University of Florida — Recently, a record-setting operating frequency of 410 GHz was reported for a CMOS circuit, fabricated using 45 nm technology. To measure the emission from this and related devices, we employed a Bruker 113v fourier transform interferometer. The radiation from an on-chip patch antenna attached to the 410 GHz push-push oscillator circuit was measured by placing the chip in the lamp housing of the interferometer. Emission was detected in the first and second harmonics of the oscillator fundamental. Power was estimated by comparison to that from quasi-blackbody sources (globar and mercury lamp). Possible applications will be discussed.

1Supported by the DOE through DE-FG02-02ER45984 and by the NHMFL.

2Now in Texas Instruments Inc.
10:36AM P27.00012 Measuring Spin-Lattice and Spin-Spin Relaxation Times Using a Continuous Wave Electron Paramagnetic Resonance Spectrometer, MICHAEL R. PAGE, M.R. HERMAN, K.C. FONG, D.V. PELEKHOV, P.C. HAMMEL, The Ohio State University — The spin-spin and spin-lattice relaxation times, known as $T_1$ and $T_2$, respectively, provide information about the spins in a material. This information can be used as an imaging technique in Magnetic Resonance methods. $T_1$ and $T_2$ can be measured by a Continuous Wave Electron Paramagnetic Resonance Spectrometer, provided the relationship between the input power and oscillating magnetic field is known. The advantage to this is that Continuous Wave Electron Paramagnetic Resonance Spectrometers are much cheaper than Pulse Electron Paramagnetic Resonance Spectrometers. The relationship between the input power and the oscillating magnetic field is determined by using a sample with known $T_1$ and $T_2$, measuring the absorption at different power levels, and fitting the distribution of absorptions to a curve. We show the results of this measurement with a Bruker EMX 2.7 Continuous Wave Electron Paramagnetic Resonance Spectrometer. This work was supported by The U.S. Army Research Office MURI under contract W911NF-05-1-0414 and by The U.S. Army Research Office DURIP under contract W911NF-07-1-0305.

10:48AM P27.00013 Terahertz Near-Field Nanoscopy of Mobile Carriers in Single Semiconductor Nanodevices, ANDREAS J. HUBER, Max-Planck-Institut für Biochemie, Munich, Germany and CIC nanoGUNE, San Sebastian, Spain, FRITZ KEILMANN, Max-Planck-Institut für Biochemie, Munich, Germany, J. WITTBORN, Infineon Technologies AG, Munich, Germany, JAVIER AIZPURUA, CSIC-UPV/EHU and DIPC, San Sebastian, Spain, RAINER HILLENBRAND, Max-Planck-Institut für Biochemie, Munich, Germany and CIC nanoGUNE, San Sebastian, Spain — We introduce ultraresolving Terahertz (THz) near-field microscopy based on THz scattering at atomic force microscope tips. Nanoscope resolution is achieved by THz field confinement at the very tip apex to within 30 nm, which is in good agreement with full electro-dynamic calculations. Imaging semiconductor transistors, we provide first evidence of 40 nm ($\lambda/3000$) spatial resolution at 2.54 THz (wavelength $\approx 118 \mu m$) and demonstrate the simultaneous THz recognition of materials and mobile carriers in a single nanodevice. We find that the mobile carrier contrast can be directly related to near-field excitation of THz-plasmons in the doped semiconductor regions. This opens the door to quantitative studies of local carrier concentration and mobility at the nanometer scale. The THz near-field response is extraordinary sensitive, providing contrast from less than 100 mobile electrons in the probed volume. Future improvements could allow for THz characterization of even single electrons or biomolecules.

Wednesday, March 18, 2009 8:00AM - 11:00AM
Session P28 FLAP: Focus Session: Thermoelectricity in Si-containing Materials 330

8:00AM P28.00001 Atomistic Simulations of Heat Transport in Silicon Nanowires, DAVIDE DONADIO, University of California Davis — Silicon is one of the best known materials of our age, cheap and readily available, being the basic constituent of semiconductor electronics. It would therefore be highly desirable to broaden its utilization for, e.g., renewable energy applications. Recently, it has been proposed that Silicon may be engineered to be an efficient thermoelectric material for use in solid state devices. Although a rather inefficient thermoelectric in its bulk form, at the nanoscale Si may become a poor heat conductor, while retaining good electronic conduction properties, and thus exhibit high efficiency in converting heat into electric current. However the fundamental reasons for the reported low heat conduction in Si nanowires (NW) are not yet understood, and different interpretations has so far appeared in the literature. Here we present atomistic simulations of heat conduction in Si NW of 1 to 3 nm diameter. Our results show that, depending on their surface structure, these wires may exhibit values of the thermal conductivity varying by two orders of magnitude, and as high as those of bulk Si. This clearly indicates that the increased surface to bulk ratio at the nanoscale may be only partially responsible for the decreased thermal conductivity observed experimentally. We also find that diffusive, yet extended, vibrational modes present in the case of wires with amorphous surfaces, are responsible for the dramatic decrease in thermal conductivity. Our findings suggest ways of engineering wires with even lower thermal conductivity, by increasing surface disorder, in particular by alloying Si with, e.g. Ge at the crystalline-amorphous interface.

1Work supported by DARPA grant W911NF-06-1-0175 and DOE/BES grant DE-FG02-06ER46262.

8:36AM P28.00002 Ultralow thermal conductivity in Electrolessly Etched (EE) Silicon Nanowires, KEDAR HIPPALGAONKAR, RENKUN CHEN, BAIR BUDAEV, Dept of Mech Eng, UC Berkeley, JINYAO TANG, SEAN ANDREWS, Dept of Chem, UC Berkeley, PADRAIG MURPHY, SUBROTO MUKERJEE, JOEL MOORE, Dept of Phys, UC Berkeley, PEIDONG YANG, Dept of Chem, UC Berkeley, ARUN MAJUMDAR, Dept of Mech Eng, UC Berkeley — EE process produces single-crystalline Silicon nanowires with rough walls. We use suspended structures to directly compute the heat transfer through single nanowires. Nanowires with diameters less than the mean free path of phonons impede transport by boundary scattering. The roughness acts as a secondary scattering mechanism to further reduce phonon transport. By controlling the amount of roughness it is possible to push limits to the extent that nanowire conductance close to quanta of thermal conductance, $hT/\pi k_B^2$ is observed. Traditionally, the lower limit of conductivity is amorphous Silicon at 1 W/mK at room temperature. The measured conductivity of our nanostructures challenges even this amorphous limit pointing towards previously unstudied mechanisms of thermal resistance. We measure thermal conductivity of ~150nm diameter EE wires to be ~1 W/mK.

1DOE, BES, A-STAR Singapore, Microlab at UC Berkeley, Molecular Foundry at Lawrence Berkeley National Labs

8:48AM P28.00003 Thermoelectric Power of Silicon Nanowires, HYUK JU RYU, DEBORAH PASKIEWICZ, SHELLEY SCOTT, MAX LGALLY, MARK ERIKSSON, UNIVERSITY OF WISCONSIN-MADISON TEAM — Thermoelectric nanomaterials have been attracting considerable interest for the cooling of hotspots and the conversion of waste thermal energy into useful electrical energy. There is special interest in silicon thermoelectrics because of potential monolithic integration on microchips as well as opportunities in nanofabrication and bandstructure engineering. We present measurements of the thermoelectric power of silicon nanowires with different doping concentrations and the gate field effect. Because silicon heterostructures can have modulation in charge density and mobility along the charge path, we have fabricated and measured silicon/silicide, silicon/silicon-germanium, and hybrid orientation silicon heterostructures in the form of nanowires. Measurements of the thermoelectric power of these structures and the effects of the internal interfaces will be presented and compared with theoretical calculations. This work is supported by DOE, AFOSR, NZ-FRST, NDSEG, NSF, and SOITECH.

9:00AM P28.00004 Thermoelectric Properties of Higher Manganese Silicide Nanowires, ARDEN MOORE, THE UNIVERSITY OF TEXAS AT AUSTIN, JEREMY HIGGINS, University of Wisconsin-Madison, FENG ZHOU, THE UNIVERSITY OF TEXAS AT AUSTIN, SONG JIN, University of Wisconsin-Madison, LI SHI, THE UNIVERSITY OF TEXAS AT AUSTIN — Higher manganese silicides (HMS) have a relatively high thermoelectric figure of merit (ZT) of about 0.7. HMS nanowires have been synthesized using a chemical vapor deposition method. In this work, the thermoelectric properties of individual HMS nanowires are measured and determined to rule the role of size effects on electron and phonon transport as well as potential ZT enhancement. Measurements of Seebeck coefficient, electrical conductivity, and thermal conductivity were performed using both suspended and substrate-based microdevices. Results show that the Seebeck coefficient of two as-synthesized 60 nm diameter nanowires between 300-400K is about 25-50% lower than that of single crystal bulk parallel to the c-axis, while the electrical conductivity values are about 25% lower than bulk single crystal in the same direction. The thermal conductivity of one 60 nm diameter nanowire at room temperature was found to be four times smaller than the bulk value along the c-axis. The large reduction in thermal conductivity and small to moderate impact on electrical transport may lead to HMS nanowires with enhanced ZT.
The enhancement of power factor is mainly due to increase in mobility of carriers without much affecting the Seebeck coefficient. We have improved onboard electrical power to several US space vehicles. Since their performance is related to dimensionless figure-of-merit (ZT), material scientists have focused on possible improvements in ZT of SiGe alloys through an increase in power factor and decrease in thermal conductivity. We have improved their attention on possible improvements in ZT of SiGe alloys through an increase in power factor and decrease in thermal conductivity. We have improved the total Seebeck coefficient in agreement with experiment. Boundary roughness scattering indeed proves to have a significant effect on both electronic and thermal transport, and we discuss a novel method to account for the phonon boundary scattering, which supplants the use of the phenomenological specular parameter. We demonstrate that indeed the room-temperature figure of merit in thin wires reaches values close to 1, and discuss options for its further enhancement.

1This project was supported by the NSF through the University of Wisconsin MRSEC, award DMR-0520527

9:48AM P28.00008 Lattice thermal conductivity of nanostructured semiconductors from atomistic simulations

We present an atomistic analysis of the thermal conductivity (k) of nanoporous silicon (np-Si) [1, 2], and we compare our results with those obtained for bulk crystalline (c-Si) and amorphous Si. We computed k using equilibrium molecular dynamics and Green Kubo relations; we then analyzed our results by solving the Boltzmann Transport Equation in the single mode relaxation time approximation, and by using an approach devised [3] to describe thermal transport in disordered semiconductors. We observe that in np-Si the phonon mean free path is reduced by up to a factor of 10 with respect to c-Si, yielding a reduction of the k of about 2 orders of magnitude. The predominant phonon scattering processes contributing to k can be modeled by the same non-perturbative [3] approach that describes thermal transport in a-Si.

1This project was supported by DARPA-W911NF-06-1-0175 and DOE/BES-DE-FG02-06ER46262.

10:00AM P28.00009 Direct Measurements of Figure-of-Merit in Amorphous Silicon-based Thermoelectric thin films

The primary challenge is to search for materials with optimized electrical transport while minimizing the thermal conductivity. Amorphous materials and their alloys are relatively new functionally important materials that demonstrate superior properties in wide range of applications such as in thermoelectricity because of their low thermal conductivity due the higher degree of disorder. Previously, we reported in plane thermal conductivity of amorphous Silicon Nitride (a-Si-N) membranes. In this talk we present our measurement technique and recent results of thermoelectric properties of thin film amorphous Si and its alloys by direct measurement of in plane thermal conductivity, thermopower and electrical conductivity on one platform and discuss the thermoelectric figure of merit.

10:12AM P28.00010 Enhancement in power factor in p-type bulk SiGe alloys

We have measured the thermal conductivity - e.g. in alloys it is lower than the binary endpoints due to increased scattering induced by strain and disorder. Understanding the thermal conductivity of complex materials is also important in other applications - from reducing hot-spot temperatures in electronic chips to better thermal-insulation materials. Here, we have calculated the thermal conductivity of silicon-germanium alloys using ab-initio density functional perturbation theory. The electronic structure of the alloy is studied with the virtual crystal approximation and the single mode relaxation time approximation; perturbation theory up to the third order provides phonon lifetimes, and disorder effects are taken into account by ensemble averages over configurations with random mass disorder. The contribution of acoustic and optical phonons to the thermal conductivity is also presented, together with the phonon mean free paths. These calculations could be used to estimate the size of the nanostructures that could reduce the thermal conductivity below bulk values through increased scattering of phonons.

9:12AM P28.00005 Thermal conductivity of silicon-germanium alloys from first-principles

We have calculated the thermal conductivity of silicon-germanium alloys using ab-initio density functional perturbation theory. The electronic structure of the alloy is studied with the virtual crystal approximation and the single mode relaxation time approximation; perturbation theory up to the third order provides phonon lifetimes, and disorder effects are taken into account by ensemble averages over configurations with random mass disorder. The contribution of acoustic and optical phonons to the thermal conductivity is also presented, together with the phonon mean free paths. These calculations could be used to estimate the size of the nanostructures that could reduce the thermal conductivity below bulk values through increased scattering of phonons.

9:24AM P28.00006 ABSTRACT HAS BEEN MOVED TO S1.00260 —
10:36AM P28.00012 High Temperature Elastic Moduli Measurements and Phase Transition Studies of Novel Thermoelectric Materials. GUANCYAN LI, RESHEED ADEBISSI, JOSH GLADDEN. University of Mississippi — Thermoelectric (TE) materials can be used to convert heat including waste heat to electrical power. They are one component to energy savings and independence. Silicon germanium (SiGe) and Zintl phase compounds are excellent candidates for high temperature applications. The mechanical properties of these materials need to be known before their actual applications in high temperature (1000°C) environments. The temperature dependent elastic moduli of five different SiGe alloys were successfully measured using a high temperature resonant ultrasound spectroscopy (RUS) technique. A linear trend is generally observed up to 600°C, a downward curvature especially in two n-type samples is noticeable at higher temperatures. Hysteresis is only observed in one of the n-type SiGe samples. Phase transitions, indicated by shifts in the natural frequencies of a Zintl sample, were observed near 792, 892, 931°C. The nature of these transitions will be discussed.

10:48AM P28.00013 Preparation and thermoelectric properties of Magnesium compounds. XI-UNU LIN, Eastern Kentucky University, GEORGE NOLAS, University of South Florida, DONGLI WANG. Semiconductor Manufacture International Corporation, Shanghai, China — We report on the synthesis and low temperature transport properties measurements of environmental-friendly thermoelectric materials Mg$_2$B$_n$Ge$_{2(n-1)}$ (B=Si, Ge, Sn) and their alloys. These semiconductors are prepared through solid-state reaction of constituent elements. The effect of electrons doping and structure vacancies on thermoelectric properties are studied by substituting trivalent Sb for tetravalent Ge or Si on Mg$_2$Si and Mg$_2$Ge compounds. For Mg$_2$B$_n$Si, both the Seebeck coefficient and electrical resistivity first decrease and then increase with increasing Sb content, whereas the thermal conductivity decrease monotonically. The Mg$_2$Si system displays similar tendency in seebeck coefficient, resistivity, and thermal conductivity but shows smaller magnitudes. Our Hall measurement at room temperature indicates that the modulation in these thermoelectric properties can be accounted for by the variance of electron concentration. The Mg$_2$Si$_{1-x}$Sn$_x$ solid solutions were prepared and investigated to study the dependence of thermoelectric properties on carrier types and carrier concentrations.

Wednesday, March 18, 2009 8:00AM - 11:00AM – Session P29 DMP GMAG: Focus Session: Manganites

8:00AM P29.00001 Recent studies of models for manganites in the bulk and in superlattices$^1$. SHUAI DONG. 1. University of Tennessee, Knoxville; 2. Oak Ridge National Laboratory; 3. Nanjing University — In this talk, we will review our recent double-exchange model studies for manganites and some related experimental discoveries. First, we will briefly address the existence of a clear CMR effect in numerical simulations, and the short-range spin and charge correlations and local density of states in this CMR regime [1, 2]. Second, we will analyze manganite superlattices (LaMnO$_{3(n+1)}$/SrMnO$_3$)$_n$. The reconstruction of charge density, spin order, and orbital order at the interfaces and the relation with a novel experimentally observed metal-insulator transition (MIT) at $n = 3$ will be discussed [3]. Finally, the multiiferroic spin order in the undoped manganite $\text{RMnO}_3$ ($R = \text{Tb}, \text{Dy}$) will be also briefly studied under the double-exchange framework [4].

$^1$Work was supported by the NSF DMR-0706020 and the Division of Materials Science and Engineering, U.S. DOE, under contract with UT-Battelle, LLC. S.D. was also supported by the China Scholarship Council.

8:36AM P29.00002 Small dissimilarity in lattice distortion triggers anomalously large anisotropic magnetoresistance in manganite perovskites$^1$. R. LI, Ningbo Institute of Materials Technology and Engineering, CAS, China; H. WANG, X.Z. WANG, Y. MATSUI. National Institute for Materials Science, Tsukuba, Japan; X. WANG. Florida International University, Miami, FL 33199, Z. CHENG, B. SHEN. Institute of Physics, CAS, Beijing 100080, China; E.W. PLUMMER, JIANDI ZHANG. Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Anisotropic magnetoresistance (AMR) effects are of fundamental importance not only for providing information on spin-orbital coupling and magneto-crystalline anisotropy, but also for enabling technological applications. Here, we report an anomalous AMR effect in a prototype manganite single crystal—$\text{La}_{0.59}\text{Ca}_{0.41}\text{MnO}_3$. We demonstrate that the broken symmetry, through cubic to orthorhombic structural distortion in the crystal, leads to profound anisotropic magneto-transport behavior. The measured AMR behavior shows a direct correlation with the anisotropic field-tuned metal-insulator transition (MIT) in the system and can be understood via a phenomenological uniaxial anisotropy model. It is revealed that a small crystalline anisotropy can trigger a large AMR near the MIT phase boundary of the system.

$^1$Supported by MEXT of Japan and the U.S. NSF DMR-0346826.

8:48AM P29.00003 Doping dependent evolution of the polaron metal. N. MANNELLA, K. TANAKA, S.-K. MO, W. YANG, H. ZHENG, J. MITCHELL, J. ZAÄÑEN, T.P. DEVERAUX, N. NAGAOSA, Z. HUSSAIN, Z.-X. SHEN. University of Tennessee-Knoxville — Experimental and theoretical evidence has already suggested that the ferromagnetic metallic (FM) phase in colossal magnetoresistive manganites is not a conventional metal but rather a polaronic conductor. In the bilayer manganites $\text{La}_{2-x}\text{Sr}_x\text{Si}_{1+2x}\text{Mn}_2\text{O}_7$ (LSMO), Angle Resolved Photoemission (ARPES) experiment revealed that the FM phase is a polaronic metal with a strong anisotropic character of the electronic excitations [1, 2]. A small but well-defined quasiparticle (QP) with heavy mass along the [110] or “nodal” direction is found to account for the metallic properties and their temperature dependent evolution [2]. In this talk, we will discuss recent ARPES results on the $x = 0.60$ composition and contrast them to the $x = 0.40$ results. Recent work has shown that the region in proximity of $x = 0.60$ constitute the most metallic bilayer manganite with DC conductivity about one order of magnitude higher than that corresponding to the region $0.30 < x < 0.40$. Much as in the $x = 0.40$ composition, for $x = 0.60$ along the nodal direction we observe a peak-dip-hump structure with QP of heavy effective mass. Quantitative differences in the electron-phonon coupling constant $\lambda$, the QP spectral weight and the hump energy are fully consistent with the doping evolution of the transport properties. [1] Nature 438, 474 (2005), [2] Phys. Rev. B 76, 233102 (2007).

9:00AM P29.00004 Metal-insulator transition in $\text{La}_{2-x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ ($x=0.59$) revealed by ARPES. ZHE SUN, J. F. DOUGLAS, Q. WANG. University of Colorado at Boulder, A. FEDOROV, Y. -D. CHUANG. Advanced Light Source, Lawrence Berkeley National Laboratory, H. ZHENG, J. F. MITCHELL. Argonne National Laboratory, D. S. DESSAU. University of Colorado at Boulder — Using angle-resolved photoemission spectroscopy (ARPES), we studied the metal-insulator transition of $\text{La}_{2-x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$ ($x=0.59$). Below $T_c$, there is significant metallic weight at the Fermi level, while a gap opens above $T_c$, in excellent agreement with resistivity measurements. We also found that in this compound the metal-insulator transition is associated with a remarkable coherent-incoherent weight transfer from the dispersive band to a non-dispersive feature over a large energy scale. The band dispersion also shows an unusual change with increasing temperature, suggesting complicated interactions in this material.
9:12AM P29.00005 Role of Oxygen Electrons in the Metal-Insulator Transition in the Manganosite Oxide La$_{2-x}$Sr$_1{+x}$Mn$_7$O$_{21}$, W. AL-SAWAI, B. BARBIELLINI, Northeastern U., (NU), A. KOIZUMI, U. Hyogo, P.E. M. JNARENDRA, Delft U. of Tech, & NU, T. NAGAO, U. Hyogo, K. HIROTA, Osaka U., M. ITOU, JASRI (SPRING-8), Y. SAKURAI, SPRING-8, A. BANSIL, NU. We have studied the [100]-[110] anisotropy of the Compton profile in the bilayer manganite. Quantitative agreement is found between theory and experiment with respect to the anisotropy in the two metallic phases (i.e. the low temperature ferromagnetic and the colossal magnetoresistant phase under a magnetic field of 7T). Robust signatures of the metal-insulator transition are identified in the momentum density for the paramagnetic phase above the Curie temperature. We interpret our results as providing direct evidence for the transition from the metallic-like to the admixed ionic-covalent bonding accompanying the magnetic transition. The number of electrons involved in this phase transition is estimated from the area enclosed by the Compton profile anisotropy differences. Our work demonstrates the sensitivity of the Compton scattering technique for identifying the number of electrons involved in the metal-insulator transition. Work supported in part by the USDOE.

9:24AM P29.00006 Charge/Orbital Ordered Phases of La$_2-2x$Sr$_1+2x$Mn$_7$O$_{21-\delta}$, KENNETH GRAY, HONG ZHENG, QING’AN LI, JOHN MITCHELL, Argonne National Laboratory — Our studies have significantly modified the conventionally-held view of the phase diagram of La$_{2-2x}$Sr$_{1+2x}$Mn$_7$O$_{21-\delta}$ for four compositions exhibiting charge (and orbital) order (CO), i.e., at hole doping levels, h=\pm 0.5 and \pm 0.6. These CO phases are stable over very narrow doping ranges (\Delta h \sim 0.005) at the lowest temperatures, but those ranges increase at higher temperatures (\Delta h \sim 0.02) in a manner consistent with simple entropy considerations. Such narrow ranges dictate the crucial need for crystal homogeneity. Attesting to such homogeneity is a conductivity ratio of \sim 10$^3$ upon crossing the first-order phase boundary from CO at h=0.60 to AAFM at h=0.59 or h=0.61 plus two findings that were missed in the existing literature: that these CO phases are the ground state at the lowest temperatures and, for h=0.5, that coexistence of the CO and AAFM phase is absent at any temperature.

1Work supported by U.S. D.O.E. under contract # DE-AC02-06CH11357.

9:36AM P29.00007 Resonant Inelastic X-ray Scattering in CE-ordered bilayer manganite, FRANK WEBER, STEPHAN ROSENKRANZ, JOHN-PAUL CASTELLAN, JOHN MITCHELL, HONG ZHENG, Materials Science Division, Argonne National Laboratory, DIEGO CASA, THOMAS GOG, X-ray Science Division, Argonne National Laboratory — Resonant Inelastic X-ray Scattering (RIXS) has recently emerged as valuable tool in the study of orbital excitations in transition metal oxides. Stephan We have performed RIXS measurements at the Mn K-edge in the half doped bilayer manganite La$_2$Sr$_2$Mn$_2$O$_7$. Our sample was a non-reentrant single crystal with long range CE order down to lowest temperatures. We made wave vector dependent energy loss scans with \Delta E=15eV in the (110) direction at three different temperatures, i.e. T=75K (AFM CE ordered), 175K (FM CE ordered), and 250K (FM and no orbital order). In particular, we compare the temperature dependence of the 2eV peak with previous results on manganite perovskites [1]. Work supported by US DOE-BES-DE-AC02-06CH11357.


9:48AM P29.00008 Time-resolved Optical Study of Charge-ordered Manganites, 1 TAKAHAJI TAKAMA, JUDY CHERIAN, RYAN DEROSA, PAULA SAHANGGAMU, SANHITA GHOSH, STEPHEN MCGILL, National High Magnetic Field Laboratory, Florida State University, TAI-TOI WANG, X-ray Science Division, Argonne National Laboratory — Charge and orbital order effects in La$_2$Sr$_2$Mn$_2$O$_7$, a complex Mott insulator with a large magnetic response, have been extensively studied since the magnetic-field induced melting of charge and orbital order (CO-OO) results in colossal magnetoresistance phenomena. However, there remain two points to be clarified, concerning the CO-OO states. First issue is the degree of charge disproportionation (CD); Full CD between Mn$^{3+}$ and Mn$^{4+}$ ions has been widely believed while charge density wave ordering with less distinct CD has also been recently proposed. Another issue is the orbital shape at critical doping levels (\sim 0.59 or h=0.61) plus two findings that were missed in the existing literature: that these CO phases are the ground state at the lowest temperatures and, for h=0.5, that coexistence of the CO and AAFM phase is absent at any temperature.

1This work was supported by the NSF-DMR-0706610 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

10:00AM P29.00009 Lattice-form dependent charge- and orbital- ordered states in perovskite-related mangananites, DAISUKE OKUYAMA, CMGR-RIKEN, YUSUKE TOKUNAGA, ERATO-JST, REJI KUMAI, AIST, YASUJIRO TAGUCHI, CMGR-RIKEN, TAKA-HISA ARIMA, Tohoku Univ., YOSHINORI TOKURA, Univ. of Tokyo — Charge and orbital order in half-doped manganites has been extensively studied since the magnetic-field induced melting of charge and orbital order (CO-OO) results in colossal magnetoresistance phenomena. However, there remain two points to be clarified, concerning the CO-OO states. First issue is the degree of charge disproportionation (CD); Full CD between Mn$^{3+}$ and Mn$^{4+}$ ions has been widely believed while charge density wave ordering with less distinct CD has also been recently proposed. Another issue is the orbital shape (OS) at Mn$^{3+}$ ion in the CO-OO phase. The reason why the OSs of (La,Ca)MnO$_x$ at hole doping levels, h=x-0.5 (PCMO) and La$_{(1-x)}$Ca$_x$MnO$_3$ (x=0.18) (LCMO) using time-resolved techniques. Our measurements are performed down to 4 K and in dc magnetic fields up to 31 T. The conductivity of the low-temperature strong charge/orbital order in PCMO is altered by the application of an electric field and a magnetic field. We demonstrate that this time-resolved optical observation is capable of capturing these mixed electronic and magnetic effects to gain further insight into the change of the ordering.

1This work was supported by the NMFH through an UCGP grant.

10:12AM P29.00010 Charge and orbital order effects in La$_2$Sr$_{1-x}$Mn$_{1+y}$O$_6$, B. DABROWSKI, Physics Department, Northern Illinois University, DeKalb, IL 60115, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, L. SUESCUN, Facultad de Quimica, Universidad de la Republica, Montevideo, Uruguay, S. KOLESNIK, S. REMSEN, J. MAIS, Physics Department, Northern Illinois University, DeKalb, IL 60115 — Low temperature annealing in hydrogen have been used to obtain oxygen vacancy ordered manganites Sr$_4$Mn$_{1+y}$O$_{10+3x}$ (n=0, 1, 3) displaying charge and orbital ordering. For the La-substituted n=1 phase four Mn$^{3+}$ cations exhibit elongated pyramidal coordination while the fifth one in octahedral coordination shows decreasing formal valence Mn$^{4-(5-\delta)}$. This selective doping produces structural strain resulting in unusual apically compressed coordination leading to complex magnetic interactions and frustration. These structures have been previously observed for the (La,Ba)CuO$_3$-$\delta$ cuprates revealing common vacancy ordering relationships in perovskites for which highly distorted Mn$^{3+}$ (Cu$^{2+}$) and symmetric Mn$^{4+}$ (Cu$^{2+}$) ions are present simultaneously. Work at NU was supported by the NSF-DMR-0706610 and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.

10:24AM P29.00011 Phase separations in La$_{1-x}$Ca$_x$MnO$_3$ at critical doping levels, J. TAO, Q. JIE, Q. LI, Y. ZHU, Condensed Matter Physics & Materials Science Department, Brookhaven National Lab, D. NIEBIESKIKWIAT, Colegio de Ciencias e Ingenieria, Universidad San Francisco de Quito, Ecuador, M.B. SALAMON, Department of Physics, University of Texas at Dallas, S.J. PENNYCOOK, Materials Science & Technology Division, Oak Ridge National Lab — La$_{1-x}$Ca$_x$MnO$_3$ specimens have been widely studied for their rich and complex physics. There is a boundary in the phase diagram at x = 0.50. At low temperatures, the system is ferromagnetic for x less than 0.5 while charge ordering phase is favored for x equal to or greater than 0.5. The mechanisms for this drastic change over the continuous doping still remains unclear. Here we report our electron diffraction study on bulk La$_{1-x}$Ca$_x$MnO$_3$ at the critical doping x = 0.48 and 0.50. Lorentz microscopy is also employed in the study to obtain the magnetic domain information during the phase transitions in these two specimens. The observed structure is integrated with the measured properties and it shows novel phenomena of the materials at nanoscale. This work is funded by U.S. DOE/BES under Contract No. DE-AC02-98CH10886.
300K up to 5 layers, but revealed strong half-order spots with weak intensity at quarter-order by 20 layers. STM images show the surfaces of thick films to have

We have measured electrical conductivity and structure of in-situ grown SRO films using scanning probe microscopy, low energy electron diffraction (LEED)

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8:48AM P30.00005 Atomic control and characterization of surface defect states of TiO2 terminated SrTiO3.\(^1\) A. KAREEV, University of Arkansas, M. KAREEV, S. PROSANDEEV, J. LIU, C. GAN, J.W. FREELAND, MIN XIAO, J. ZHANG, L. BRILLSON, J. CHAKHALIAN — By using a new wet-etch procedure\(^1\) we have obtained high-quality atomically flat TiO2 terminated surfaces of STO (100) single crystals with the surface morphology equivalent or better to that of the conventional routes. By applying a combined power of CL and PL, RHEED, AFM, and resonant XAS, we are able to identify and monitor the complex evolution of oxygen defect states and Ti ion valency at the surface and near-surface regions. Our data reveal a high level of local defects resulting in the presence of the Ti\(^{3+}\) states at the surface in the conventionally treated STO surface. We have developed an efficient method to control the defect states capable of a marked reduction of the defect concentration. We have demonstrated that the PL, CL and XAS are able to distinguish the surface-related Ti states from oxygen vacancies trapping charge transfer vibronic excitons. \(^1\)M. Kareev et al., Appl. Phys. Lett. 93, 061909 (2008).

Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357. J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.

9:00AM P30.00006 Polar and non-polar oxide interfaces: charge and spin behaving badly\(^1\). WARREN PICKETT, UC Davis — Interfaces between two dissimilar materials are well known to lead to new behavior and often useful properties. Whereas covalent semiconductors have been studied and used for decades, and the interfaces of magnetic metals also have assumed great importance, the use of oxides in such juxtaposed systems is much more recent. Oxides add the huge impact of ionicity, and the correlated electron behavior that occurs if open shells are present. Even without correlation effects, finite overlayers (slabs) involving a polar discontinuity can sustain a surprisingly large separation of charge, as will be illustrated with calculational results on LaAlO\(_3\) slabs on SrTiO\(_3\) substrates: a strong polar distortion, uniform over several unit cells, creates the necessary screening. The most recent results on the mechanism and character of the insulator-to-metal transition with thickness will be discussed. Polar discontinuities are not necessary to create exotic behavior, as we illustrate with rutile-structure VO\(_2\)/TiO\(_2\) multilayers, where a topologically protected zero-gap two-dimensional half-metal arises in a thickness regime between thin insulating and thick conducting VO\(_2\) slabs. Work done in collaboration with R. Pentcheva, V. Pardo, and K. Ott.

\(^1\)Supported by a Bavaria California Technology Center grant, the France-Berkeley Fund, and DOE/BES.

9:36AM P30.00007 Prediction of a switchable two-dimensional electron gas at KNbO3/ATiO3 (A = Sr, Ba, Pb) interfaces, YONG WANG, MANISH NIRANJAN, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska, Lincoln NE, USA — The demonstration of a quasi-two dimensional electron gas (2DEG) at the (LaO\(^+)/\((/TiO2)\(^0\)) interface in LaAlO\(_3\)/SrTiO\(_3\) heterostructure has fuelled intense research activity in recent years. The 2DEG has a high carrier mobility and electron density that are promising for applications in all-oxide electronic devices. For such applications it is desirable to have the ability to control the properties of the 2DEG by external stimulus, e.g., by an electric field. In this study we use density functional calculations to explore a ferroelectric KNbO\(_3\)/SrTiO\(_3\) heterostructure for this purpose. The polar discontinuity at the (NbO\(_2\))\(^+)/\((/SrO)\(^0\))interface in KNbO\(_3\)/SrTiO\(_3\) heterostructure is similar to that at the (LaO\(^+)/\((/TiO2)\(^0\)) interface in LaAlO\(_3\)/SrTiO\(_3\) heterostructure. Our results suggest that a 2DEG is created at the (NbO\(_2\))\(^+)/\((/SrO)\(^0\))interface due to the electronic reconstruction with properties strongly determined by the orientation of the electric polarization. We further explore the formation of 2DEG at the interfaces of all ferroelectric KNbO\(_3\)/BaTiO\(_3\) and KNbO\(_3\)/PbTiO\(_3\) heterostructures and its dependence on polarization orientation. Finally, we discuss how the properties of 2DEG in aforementioned heterostructures are influenced by the compensation of polarization charges by free carriers, rendering it switchable.

9:48AM P30.00008 A Novel Quantum Well of Embedded SrTiO\(_3\) in LaAlO\(_3\), HANGHUI CHEN, ALEXIE KOLPAK, SOHRAB ISMAIL-BIEGI, Department of Physics, Yale University — Inspired by the novel behavior of LaAlO\(_3\)/SrTiO\(_3\)(001) heterointerfaces, we propose new sets of interfaces in which one TiO\(_2\) or SrO layer is embedded in LaAlO\(_3\). These interfaces can form quantum wells which trap electrons or holes in a single atomic layer of TiO\(_2\) or SrO, respectively, when the “polar catastrophe” occurs. This narrow confinement, in contrast to the situation at the LaAlO\(_3\)/SrTiO\(_3\)(001) interfaces, sheds light on the still uncertain origin of the charge carriers and provides ideas for engineering their properties. In addition, we study the field effect on these systems to predict the critical external electric field required to induce an insulating-to-metallic transition.

10:00AM P30.00009 Resonant Tunneling Through a Two-Dimensional Electron Gas in All-Oxide Heterostructure Tunnel Junctions, J.D. BURTON, E.Y. TSYMBAL, University of Nebraska, Lincoln, USA, J.P. VELEV, University of Puerto Rico, San Juan, USA — Oxide heterostructures exhibit a variety of very interesting physical properties and have tremendous potential for new types of multifunctional device applications. For example, very recently it was discovered that a two-dimensional electron gas (2DEG) is formed at the (001) interface between two perovskite oxides that are otherwise insulating in the bulk. We examine, within the framework of first-principles density functional theory, the effect of a complex SrTiO3-LaO-SrTiO3 barrier forming a 2DEG on conductance and TMR in all-oxide magnetic tunnel junctions. The replacement of one SrO atomic layer by LaO in the otherwise pure SrTiO3 barrier can be understood as precision substitutional doping of trivalent La for divalent Sr, leading to the formation of a 2DEG. Such precision atomic layering is within the reach of current experimental fabrication techniques. Our calculations reveal that the pure SrTiO3 barrier, the tunneling conductance can be substantially enhanced due to resonant tunneling through the 2DEG. However, this effect is sensitive to lattice polarization effects in the SrTiO3 barrier as well as the choice of electrode material. We will discuss these effects with the goal of stimulating experimental studies.

10:12AM P30.00010 Modulation of the low-temperature magnetoresistance of Ar-irradiated SrTiO\(_3\) via field-effect gate doping, J.H. NGAI, Department of Applied Physics, Yale University, Y. SEGAL, J. HOFFMAN, F.J. WALKER, C.H. AHN, CENTER FOR RESEARCH ON INTERFACE STRUCTURES AND PHENOMENA TEAM — Recent experiments have shown that irradiating single crystal SrTiO3 with Ar ions can create an amorphous surface layer with a quasi-2-dimensional electron gas (Q2DEG) below. We present low-temperature magnetotransport measurements of this Q2DEG system, as a function of gate doping. The magnetoresistance can be tuned as n-type carriers are doped into the interface between the amorphous and crystalline SrTiO3 layers. Anisotropy in the magnetoresistance is also measured with respect to the direction of the applied magnetic field. These results will be compared with the magnetotransport properties of LaAlO\(_3\)/SrTiO3 heterostructures, where the possibility of novel magnetic behavior will be discussed.
10:24AM P30.00011 Nanoscale Electrical Properties of Oxide Heterostructures Revealed Via Introspection\(^1\). CHENG CEN, STEFAN THIEL, JOCHEN MANNHART, JEREMY LEVY — Previous work shows that conductive regions can be formed via lateral nanoscale confinement of a quasi-two-dimensional electron gas at the LaAlO\(_3\)/SrTiO\(_3\) interface\(^2\). Here we demonstrate how structures constructed in this method serve not only as novel nanoelectronic devices but also as tools for studying fundamental physics in the underlying material system. Nanowires, tunnel junctions, field effect transistors (FETs), together with associated phenomena that we observed such as negative differential resistance, provide insight into the mechanism responsible for the existence and spatial confinement of the interfacial metal-insulator transition. We discuss several examples of nanodevices and the constraints they place on models and mechanisms that govern their properties. \(^2\)Cen et al, Nature Materials 7, 298 (2008).

\(^1\)This work was supported by NSF-0704022, the DFG (SFB 484), and the EC (Nanoxide).

10:36AM P30.00012 A metal-insulator transition tunable by lattice deformation in LaTiO\(_3\) thin films\(^1\), FRANKLIN WONG, University of California, Berkeley, SEUNG-HYUB BAEK, HO WON JANG, University of Wisconsin, Madison, RAJESH CHOPDEKAR, VIRAT MEHTA, University of California, Berkeley, CHANG-BEOM EOM, University of Wisconsin, Madison, YURI SUZUKI, University of California, Berkeley — Strong electron-electron and electron-lattice correlations play critical roles in electronic transitions of complex oxides. LaTiO\(_3\) is a narrow bandgap Mott insulator on the verge of a metal-insulator transition, substrate-induced lattice distortions offer a route to tuning its electronic properties. We have observed metallic to insulating behavior in LaTiO\(_3\) films depending on choice of (001) substrates: SrTiO\(_3\), LSAT, and LaAlO\(_3\). Tetragonal distortions induced by epitaxial in-plane compression from the SrTiO\(_3\) substrates result in metallicity in LaTiO\(_3\) films, while films on LSAT substrates exhibit a range of electronic properties depending on the degree of lattice relaxation. Whereas thinner LaTiO\(_3\) films on LSAT exhibit “semimetallic” behavior, in thicker films, the out-of-plane lattice parameters surprisingly converge to values greater than the bulk lattice constant, and the films become more insulating. We will discuss the profound consequences thin-film lattice deformation has on electrical transport. We speculate that stabilization of lattice distortions via epitaxy may open a new avenue for materials engineering of oxides through careful control of structural perturbations.

Wednesday, March 18, 2009 8:00AM - 11:00AM – Session P31 GMAG: Focus Session: Spin Ice 335

8:00AM P31.00001 Magnetothermodynamics of spin ice and related compounds\(^1\). XIANGLIN KE, The Pennsylvania State University — Geometrically magnetic frustration, which results from the competition of spin-spin interactions of magnetic ions on a regular magnetic lattice, leads to a variety of exotic low temperature states including “spin ice.” “Spin ice” refers to a magnetic state wherein the two-in-two-out spin configurations of rare earth pyrochlore compounds mimic the proton positions in the water ice, characterized by the “zero point entropy” of (R/2) \(\ln(2)\). In this study, we examine how structural disorder affects spin dynamics and the magnetic “zero point entropy.” By diluting the “spin ice” materials with nonmagnetic ions on the rare earth sites, we have found that the entropy of the diluted species depends non-monotonically on the dilution concentration, and we explain this behavior using a generalized Pauling approximation. Nonmagnetic doping on B sites leads to only a small decrease of the “zero point entropy,” indicating the robust nature of “spin-ice.” We have also studied Dy2Ge2O7, which has the same chemical formula as “spin ice” materials and Ising-like spins but a tetragonal structure. Dy2Ge2O7 undergoes a long range antiferromagnetic ordering transition, but the spin dynamics at temperatures above the order transition is similar to that observed in the canonical “spin ice” systems, suggesting that such dynamics are generic to a broader class of Ising-like rare earth systems.

References:

\(^1\)In collaboration with B. G. Ueland, R. S. Freitas, D. V. West, G. C. Lau, M. L. Dahlberg, E. Morosan, J.A. Fleitman, R. J. Cava, R. Moessner, P. Schiffer, and supported by NSF.

8:36AM P31.00002 Magnetic charge order in kagome spin ice with dipolar interactions\(^1\). GIA-WEI CHERN, University of Wisconsin - Madison, PAULA MELLÁDO, OLEG TCHERNYSHYOV, Johns Hopkins University — Dipolar interactions in spin ice are described most effectively in terms of magnetic charges residing on the dual lattice \([1]\). While spin ice on the pyrochlore lattice contains no magnetic monopoles at low temperatures, spin ice on kagome \([2]\) contains a unit magnetic charge \((\pm 1)\) on every triangle. With the aid of Monte-Carlo simulations, we show that long-range Coulomb interaction between the monopoles lifts the degeneracy of the spin-ice states and induces a phase transition into a state with ordered magnetic charges but no spin order. The residual entropy is reduced from the spin-ice value but remains extensive. The phase transition is continuous with critical exponents close to the two-dimensional Ising universality class. \([1]\) C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature 451, 42 (2008). \([2]\) A. S. Wills, R. Ballou, and C. Lacroix, Phys. Rev. B 66, 144407 (2002).

\(^1\)Work supported in part by NSF Grant DMR-0348679.

8:48AM P31.00003 Comparing artificial frustrated magnets: geometric effects in nanomagnet arrays\(^1\), JIE LI, XIANGLIN KE, The Penn State Univ, CRISTIANO NISOLI, Los Alamos National Lab, PAUL LAMMIERT, VINCENT CRESPi, PETER SCHIFFER, The Penn State Univ — We have studied arrays of single-domain ferromagnetic islands arranged on lattices such that the magnetostatic interactions between the islands are frustrated by the geometry of the arrays. We compare results for the different lattice geometries: the previously studied square “artificial spin ice” lattice\([1,2]\), a hexagonal lattice, and a ladder lattice which is topologically-equivalent to the former one. After the ac demagnetization the magnetic moment configurations are imaged via Magnetic Force Microscopy (MFM). We find that the ladder lattice shows local correlations which are similar to those of the square lattice, suggesting it as basis for comparison of the energetics of the other two lattices. The normalized magnetostatic energy of all three geometries decreases with decreasing demagnetization step size, but the lattices approach their ground states at different rates. 1. R. F. Wang, C. Nisoli, R. S. Freitas, J. Li, W. McConville, B. J. Cooley, M. S. Lund, N. Samarth, C. Leighton, V. H. Crespi, and P. Schiffer, Nature 439, 303 (2006). 2. X. Ke, J. Li, C. Nisoli, P. E. Lammiert, W. McConville, R. F. Wang, V. H. Crespi, and P. Schiffer, Phys. Rev. Lett. 101, 037205 (2008).

\(^1\)This research is supported by the Army Research Office.
9:00AM P31.00004 Cooperative Paramagnetic Behavior in the Stuffed Pyrochlore Tb$_{2-x}$Ti$_x$Nb$_2$O$_7$. B.G. UELAND, J.S. GARDNER, NIST Center for Neutron Research, National Institute of Standards and Technology, M.L. DAHLBERG, P. SCHIFFER, Department of Physics and Materials Research Institute, Pennsylvania State University, A.J. WILLIAMS, J.C. KIM, R.J. CAVA, Department of Chemistry and Princeton Materials Institute, Princeton University — The pyrochlore Tb$_2$Ti$_2$O$_7$ is a cooperative paramagnet that has generated much interest in the frustrated magnetism community due to the presence of persistent short range spin-spin correlations and its apparent lack of long range magnetic order down to temperatures below $T = 0.05$ K, despite an effective spin-spin interaction strength given by $\theta_{V} \sim 10$ K. Motivated by recent work on the stuffed spin ices, we have begun investigations into stuffed variants of Tb$_2$Ti$_2$O$_7$, in which we replace some of the nonmagnetic Ti$^{4+}$ with magnetic Tb$^{3+}$, thus gradually altering the geometry of the magnetic sublattice from a lattice of corner sharing tetrahedra to a disordered lattice of side sharing tetrahedra. Here, we present results from magnetization and neutron scattering studies on powder samples of Tb$_{2-x}$Ti$_x$Nb$_2$O$_7$, where $x = 0$.2.0, 0.6, or 1, where diffraction data indicate that the $x = 1$ material has a disordered fluorite lattice. Preliminary results indicate that short range magnetic correlations similar to those present in Tb$_2$Ti$_2$O$_7$ exist in all of the materials studied, and that long range antiferromagnetic order may exist in the $x = 1$ material.

9:12AM P31.00005 Quantized Berry phase and entanglement entropy for a spin ladder system. ISAO MARUYAMA, Osaka university, SHOU TANAYA, MITSUHIRO ARIKAWA, YASUHIRO HATSUGAI, University of Tsukuba — We have demonstrated that quantized Berry phases and entanglement can be used as a new tool for exploring gapped systems which do not exhibit symmetry breaking. Especially, using quantized Berry phases in several gapped systems we identified location of singlet pairs successfully which illustrate the valence bond solid (VBS)[1], the itinerant singlet [2], the Kondo singlet. Recently, we have studied four-spin ring exchange interaction in a spin-1/2 two-leg ladder, which introduces frustration and generates various phases, such as the dominant vector-chirality (DVC) phase. In the DVC phase, the Berry phase detects the plaquette singlet[3] while entanglement entropy shows that degree of freedom of the edge state is non-zero. It means that singlets are localized at every links and separated as a free spin by adopting the boundary as in the VBS phase. In fact, under the open boundary condition, we found $S=1$ three-fold degenerated excited states with the small gap depends on the system-size as in the Kennedy triplet. [1] T.Hirano, H.Katsura, Y.Hatsugai, PRB 77 (2008) 094431 [2] I.Maruyama, Y.Hatsugai, JPSJ 76 (2007) 113601 [3] I.Maruyama, T.Hirano, Y.Hatsugai, AX.0806.4416

9:24AM P31.00006 Tuning magnetic frustration of nanomagnets in triangular-lattice geometry. X. KE, J. LI, S. ZHANG, C. NISOLI, V. CRESPI, P. SCHIFFER, The Pennsylvania State University — We study the configuration of magnetic moments on triangular lattices of single-domain magnetic islands, examining the consequences of magnetostatic interactions in this frustrated geometry. By varying the island-island distance along one direction, we are able to tune the ratio of different interactions between neighboring islands, resulting in a corresponding variation in the local correlations between the island moments. Unlike other artificial frustrated magnets, this lattice geometry displays regions of ordered moment orientation, possibly resulting from a higher degree of anisotropy leading to a reduced level of frustration. Reference: X. Ke et al., Appl. Phys. Lett., in press (2008).

1 We acknowledge the financial support from Army Research Office and the National Science Foundation MRSEC program (DMR-0820404) and the National Nanotechnology Infrastructure Network.

9:36AM P31.00007 Magnetization Reversal in Artificial Kagome Ice. STEPHEN DAUNHEIMER, YI QI, TODD BRINTLINGER, University of Maryland, PAULA MELLADO, OLEG TCHERNYSHYOV, Johns Hopkins University, JOHN CUMINGS, University of Maryland — Lorentz-force images of magnetic domains in artificial kagome ice in detail. Previously, no ice rule violations have been observed in this novel magnetic metamaterial [1], in contrast to artificial square ice, where ice rule violations appear to be a robust feature [2]. Theoretical considerations support this observation but predict the generation of transient defects violating the ice rules during magnetization reversal. Such defects are expected to self-annihilate upon completion of the reversal process or removal of the artificial magnetic field. We will present results on the experimental exploration for ice-rule violations in this system both during field rotation and uniaxial field reversal using both FMR and LTEM. [1] Y. Qi et al., Phys. Rev. B 77, 094418 (2008) [2] X. Ke et al., Phys. Rev. Lett. 101, 037205 (2008)

1This work was supported by NSF DMR-0705368 and NSF-MRSEC (DMR 0520471).

9:48AM P31.00008 Equilibration and response properties in spin ice systems. CLAUDIO CASTELNOVO, University of Oxford, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, SHIVAJI SONDHI, Princeton University — It was recently argued that magnetic monopoles emerge in a class of exotic magnets known as spin ice: the dipole moment of the underlying electronic degrees of freedom fractionalises into deconfined monopoles. Here we investigate analytically and numerically the effects that these peculiar excitations have on the equilibration and response properties of a system. In particular, we study temperature quenches in exhaustive detail. The implications of these results on the possibility of finding new experimental signatures of magnetic monopole excitations in rare earth titanates (Dy$_2$Ti$_2$O$_7$ and Ho$_2$Ti$_2$O$_7$) are discussed.

10:00AM P31.00009 Monopole and Dirac string constrained Dynamics in Spin Ice. LUDOVIC JAUBERT, PETER HOLDSWORTH, Ecole Normale Superieure de Lyon — Since its discovery approximately 10 years ago [1], spin ice has proved to be an abounding source of exotic collective phenomena, in particular long-range dipolar correlations and unconventional phase transitions. But its most impressive property is undoubtably the geometry of its fractionalized excitations. These elude simple classification, behaving like effective magnetic monopoles [2]. I shall present an experimental signature of their influence in magnetic relaxation measurements for a spin ice material Dy$_2$Ti$_2$O$_7$ [3] and show that the observed low temperature dynamical slow down can be explained quantitatively by the Coulomb interactions between monopoles and the overlapping of Dirac strings filling the quasi-particle vacuum [4].


10:12AM P31.00010 Slow spin relaxation in dipolar spin ice. MARTIN ORENDA, LUCIA SEDLAKOVA, ALZBETA ORENDACOVA, PETER VRABEL, ALEXANDER FEHER, P. J. Šafarík University and Inst. Exp. Physics SAS, Košice, Slovakia, DANIEL M. PAJEROWSKI, JUSTIN D. COHEN, MARK W. MEISEL, Dept. Physics, Univ. Florida, FL; MASAE SHIRAI, STEVEN T. BRAMWELL, Univ. College London, UK — Spin relaxation in dipolar spin ice Dy$_2$Ti$_2$O$_7$ and Ho$_2$Ti$_2$O$_7$ was investigated using the magnetocaloric effect and susceptibility. The magnetocaloric behavior of Dy$_2$Ti$_2$O$_7$ at temperatures where the orientation of spins is governed by “ice rules” ($T \ll T_{ic}$) revealed thermally activated relaxation; however, the resulting temperature dependence of the relaxation time is more complicated than anticipated by a mere extrapolation of the corresponding high temperature data [1]. A study of Ho$_2$Ti$_2$O$_7$ was performed at $T > T_{ic}$ and in high magnetic fields, and the results suggest a slow relaxation of spins analogous to the behavior reported in a highly polarized cooperative paramagnet [2]. [1] J. Snyder et al., Phys. Rev. Lett. 91 (2003) 102701. [2] B.G. Ueland et al., Phys. Rev. Lett. 96 (2006) 027216.

1Work supported by ESF-RNP-HFM, NSF DMR-0701400.
10:24AM P31.00011 Quantum Spin Ice for Pr Pyrochlore Magnets, SHIGEKI ONODA, YOICHI TANAKA, Condensed Matter Theory Laboratory, RIKEN — We theoretically propose a new state comprising a quantum-mechanical analogue of the spin ice for pyrochlore magnets. In classical spin-ice systems like Dy2Ti2O7, the ice rule is mainly driven by the magnetic dipolar interaction, which is proportional to the square of the total angular momentum J. Therefore, for Pr3+ ions having two f electrons forming the J = 4 localized moment, the dipolar interaction becomes an order of magnitude smaller than that for Dy ions. Then, the magnetic superexchange interaction should play an important role. In fact, the form of the exchange interaction is nontrivial because of the highly relativistic nature of f electrons with strong LS coupling and crystal-field effect. Here, we present a microscopic derivation of the effective relativistic spin-orbital Hamiltonian for the pyrochlore magnets Pr2Ti2O7 with a transition-metal element T. Then, it is shown that the nearest-neighbor exchange interaction is significantly modified from antiferromagnetic to ferromagnetic by quantum–mechanical processes through excited states split by the crystal field. This bears a quantum-mechanical formation of the ice rule for Pr magnetic moments. Solving the Hamiltonian for a Pr2O4 tetrahedral cluster, we obtain a further small energy splitting of the low-energy states, leaving doubly degenerate ground states per tetrahedron. Implications for the lattice model and possible relevance to experiments are also discussed.

10:36AM P31.00012 SrEr2O4 in an applied magnetic field—a quantum phase transition?, O.A. PETRENKO, G. BALAKRISHNAN, T.J. HAYES, University of Warwick, UK, P. MANUEL, D.T. ADROJA, L.C. CHAPON, ISIS, RAL, UK — SrEr2O4 belongs to a family of materials with the formula SrLn2O4, where Ln = Gd, Dy, Ho, Er, Tm and Yb. In these compounds the magnetic Ln ions are linked through a network of triangles and hexagons [1]. Despite the strong exchange interaction (θcW = ~12 K), long range ordering develops in SrEr2O4 only at 0.75 K [2]. The structure consists of FM chains running along the c axis, two adjacent chains being stacked antiferromagnetically. The moments point along the c direction, but only one of the two Er sites has a sizeable moment of 4.5 μB. An unusual behaviour in SrEr2O4 is observed in an applied field, where for Halce, a field of 0.5 T completely destroys long range magnetic order and introduces instead some sort of state with short range magnetic correlations. This conclusion is reached on the basis of neutron diffraction experiment at ISIS, where a replacement of the sharp Bragg peaks by broad diffuse scattering features is observed. A further increase in magnetic field causes a restoration of the long range order and a disappearance of the diffuse scattering. These observations resemble the behaviour seen around a quantum critical phase transition, although additional investigations are required to prove the presence of a QCP in SrEr2O4. [1] H. Karunadasa et al., Phys. Rev. B 71, 144414 (2005). [2] O.A. Petrenko et al., Phys. Rev. B 78, 184410 (2008).


8:36AM P32.00002 Magnetic and magnetotransport properties of organic trilayers of alkanedithiol self-assembled monolayers sandwiched between ferromagnetic thin films, WILLIAM RICE, JEREMY NISKALA, JEFF HALLER, PAUL HOERTZ, WEI YOU, FRANK TSUI, University of North Carolina at Chapel Hill — Magnetic and magnetotransport properties of organic spin valve structures have been studied. The organic trilayer structure consists of a self-assembled monolayer (SAM) of alkanedithiol sandwiched between two ferromagnetic metal contacts, a Ni film as the bottom contact and a Co film as the top contact. The SAM was formed using novel methods on the Ni surface on the bottom of the vertical structure. Two alternative designs have been developed, one uses an additional conducting polymer layer for electrical isolation during thermal evaporation of the top Co contact and another uses nanotransfer printing to directly apply the top Co contact. Each trilayer was examined in vacuum using 4-terminal transport measurements. Both designs have indicated tunneling as the transport mechanism between contacts. Magnetooptic Kerr Effect (MOKE) measurements show independent switching of the ferromagnetic layers at approximately 50 and 100 Gauss. Magnetotransport measurements were carried out as a function of bias voltage, temperature and field, in order to explore spin-dependent transport through the organic interlayer.

8:48AM P32.00003 Effects of interface microstructure on magnetotransport in organic spin valve structures1, YAOHUA LIU, TAEKWON LEE, M.E. KATZ, D.H. REICH, The Johns Hopkins University, S.M. WATSON, J.A. BORCHERS, NIST Center for Neutron Research — Organic semiconductors hold promise for spintronics because of their potentially long spin diffusion length. We have studied Fe/Alq3 (tris-(8-hydroxyquinoline) aluminum)/Co multilayer films with Alq3 thickness in the range 50 to 150 nm.[1] Similar to previously reported results, we found considerable variability in the magnetotransport properties for cross junctions made in nominally identical conditions. To explore the sources of these effects, we studied the microstructure of such multilayer films by X-ray reflectometry and polarized neutron reflectometry (PNR). We found that the films show well-defined layers with limited chemical intermixing (3-5 nm) at the Alq3/ferromagnet (FM) interfaces. However, larger magnetoresistance (MR) is associated with sharper Alq3/FM interfaces, and with a magnetically dead Fe-rich region at the Alq3/Fe interface, which may potentially circumvent the resistivity mismatch problem. The PNR data also show that the Co layer on top of the Alq3 can adopt a multi-domain magnetic structure at low field and a perfect anti-parallel state is not obtained. [1] Y. Liu et al., arXiv:0810.0289v1.

1Supported in part by DOE, AFOSR, and NSF.

1Work Supported by NSF Grant No. DMR-0520491.
9:00AM P32.00004 Enhanced Magnetoresistance in Alq3-based spin valve using buffer-layer assisted growth1, DALI SUN, Oak Ridge National Laboratory / Institute of Physics, Chinese Academy of Sciences, CHENGJUN SUN, LIFENG YIN, HANGWEN GUO, ZHENG GAI, XIAOGUANG ZHANG, Oak Ridge National Laboratory, ZHAO-HUA CHENG, Institute of Physics, Chinese Academy of Sciences, JIAN SHEN, Oak Ridge National Laboratory / The Univ. Tennessee — In the field of organic spintronics, interfacial diffusion between magnetic electrodes and organic spacer layers is a serious problem for both understanding the underlying mechanism and achieving high magnetoresistance. Using buffer layer assist growth, we have successfully fabricated vertical organic spin valves with much sharper interface. Spin valves prepared by this method exhibit considerably larger magnetoresistance. The spacer layer thickness-dependent magnetoresistance suggests that field-dependent interfacial barrier plays the crucial role for the observed magnetoresistance.

1Supported by the Division of Materials Science and Engineering, U. S. DOE.

9:12AM P32.00005 Spin and Charge Injection and Transport in Ferromagnet/Organic Semiconductor/Ferromagnet Heterojunction1, JUNG-WOO YOO, Department of Physics, The Ohio State University, H. W. JANG, C. B. EOM, Department of Materials Science and Engineering, University of Wisconsin-Madison, CHI-YUEH KAO, Department of Chemistry, The Ohio State University, A. J. EPSTEIN, Department of Physics and Chemistry, The Ohio State University — We studied the spin injection and transport in organic semiconductor by employing LSMO and Fe as an anode and cathode in hybrid spin valve structure. Using thin layer (t < 10 nm) of rubrene as a spacer, our device displays MR as high as 50 % at low temperature and at low bias voltage. The charge injection into organic spacer in our devices is injection limited. At high applied voltage (V > Vth) field-driven current prevails in current density through the organic semiconductor. At low bias V, inelastic hopping followed by thermionic emission is dominant at high T, which decreases significantly as T lowered. And eventually the current density through the device becomes purely tunneling at low T and V. The spin and charge injection, effects of inclusion of tunneling barrier, and the effects of crystallinity of organic layer will be discussed.

This work was supported in part by the DOE Grants No. DE-FG02-01ER45931, DE-FG02-86ER45271, AFOSR Grant No. FA9550-06-1-0175, and NSF Grant No. DMR-0805220

9:24AM P32.00006 Spin filtering of Photo-excited charge from Organic Nanostructures1, ADITYA MOHITE, BRUCE ALPHENAAR, University of Louisville, TIFFANY SANTOS, JAGADEESH MOODERA, MIT, MIT COLLABORATION — In organic materials, coupling between the incident photon and the electron spin is very weak. Here we demonstrate that spin filtering materials can be used to induce intersystem crossing, and allow the spin polarized triplet excitonic states to be probed. A thin layer of EuS was deposited at the interface formed between a single-wall nanotube and an aluminum contact. EuS is a “spin filtering material,” a ferromagnetic insulator with large spin-orbit coupling, allowing preferential tunneling by electrons of a preferred spin direction. A small magnetic field is applied to align the electron spin in the EuS with the carbon nanotube. The enhanced spin-orbit interaction allows for observation of a low-energy peak in the capacitive photocurrent scan. The energy spacing between the two peaks matches closely with the theoretical predictions for the S−T1 spacing in nanotubes. Further measurements of the triplet peak reveal that its magnitude depends on the orientation of the B-field with maximum peak occurring when the spins in EuS line up with the nanotube axis. These measurements suggest that introduction of a spin filtering layer could be used to study the triplet formation in organic solar cell materials.

1Supported by ONR N00014-06-1-0228.

9:36AM P32.00007 Spin and charge transport study in single crystal organic semiconductors1, KARTHIK V. RAMAN, CARLIJN L. MULDER, MARC A. BALDO, JAGADEESH S. MOODERA, MIT — Spin transport studies in amorphous rubrene films have shown exciting and promising results [1]. A large spin diffusion length in these amorphous films has increased the motivation to perform spin transport study in high purity single crystal rubrene. This will provide the fundamental understanding on the spin transport behavior in OS; not influenced by defects or traps. We will present work on small channel single crystal rubrene FET device with magnetic electrodes. For example, our preliminary studies have show mobility for FET with Co electrode to be 0.014cm²/V-s. A study on the spin and charge transport properties in single crystals of OS with magnetic electrodes is being done and the results will be reported. The influence of gate voltage and applied magnetic field on the transport properties will be discussed. [1] J.H. Shim et al., PRL 100, 226603 (2008)

1This work is supported by ONR, NSF and KIST-MIT project.

9:48AM P32.00008 Inter-Molecular Spin-Orbital Coupling Effects on Magnetoresistance and Spin-Dependent Excited Processes in Organic Semiconductors1, LIANG YAN, BIN HU, University of Tennessee — A low magnetic field can change electrical current and electroluminescence in organic semiconductors, leading to magnetoresistance and magnetic field effects due to magnetic field-dependent singlet/triplet ratio involved in charge transport and excited states. In general, an external magnetic field can change singlet and triplet ratios through two major pathways: spin-dependent electron-hole pairing and field-dependent intersystem crossing. We found that tuning inter-molecular spin-orbital coupling leads to a significant change in magnetoresistance, electro-fluorescence, and electro-phosphorescence. These experimental findings indicate that (i) inter-molecular and intra-molecular electron-hole pairs account for magnetoresistance and magnetic field effects, respectively, (ii) spin mixing occurs in inter-molecular excited states, and (iii) spin-mixing is a function of both spin-orbital coupling and singlet-triplet energy difference. This presentation will discuss the effects of magnetic field on both spin-dependent electron-hole pairing and spin mixing in magnetoresistance and magnetic field effects in organic semiconductors.

10:00AM P32.00009 Magnetoresistance in the High Magnetic Field Regime for Organic Semiconductors1, J. L. MARTIN, V. N. PRIGODIN, J. D. BERGESON2, Dept. of Physics, The Ohio State University, C.Y. KAO, Dept. of Chemistry, The Ohio State University, A.J. EPSTEIN, Dept. of Physics and Dept of Chemistry, The Ohio State University — While there has been much study of the low field (of order 100 Oe) magnetoresistance in organic semiconductor (OSC) materials, very little has been done in high fields of order 10kOe. Magnetoresistance studies in the high field were conducted on the OSC materials tris-(8-hydroxyquinoline) aluminum (Alq3) and alpha sexithiophene (α-6T). The high field shows a different response from that of the low field and displays several features suggesting that multiple mechanisms are at work. In addition, the two materials demonstrate behaviors that differ from one another, suggesting different classes of OSC. The experimental results are discussed in the context of the MIST model [1], which attributes magnetoresistance to the recombination of electron-hole pairs with interconversion of singlets and triplets.


1Supported in part by NSF and DOE.

2Currently at NREL.
10:12AM P32.00010 Iron Nanoparticle Driven Spin-valve Behavior in Aligned Carbon Nanotube Arrays* — MARK B. MURPHNEY, JEREMY D. BERGESON, STEPHEN J. ETZKORN, The Ohio State University, Columbus, Ohio 43210-1117, LIANGTI QU, JUNQING YANG, LIMING DAI, University of Dayton, Dayton, Ohio 45469-0246, ARTHUR J. EPSTEIN, The Ohio State University, Columbus, Ohio 43210-1117 — Spin-valve structures have been constructed from aligned arrays of carbon nanotubes, yielding a magnetoresistance reaching 25%. In addition to including vertically aligned carbon nanotube arrays, iron catalyst nanoparticles that form the array function as the second ferromagnetic electrode. Reversal of the magnetization of the electrode in an applied magnetic field results in a clear peak in the resistance of the device. A spin scattering length in excess of 9 µm shows excellent spin transport through the nanotube array. The effect of oxide barriers and device patternability are explored. 1. Bergeson, et al., Appl. Phys. Lett. 93, 172505 (2008) *This work is supported in part by DOE Grant Nos. DE-FG02-08ER45871 and DE-FG02-01ER45931, and AFOSR Grant No. FA9550-06-1-0175 and FA9550-06-1-0384, NSF Grant No. CMS-0609077, and IMR Grant Nos. FG0004 and FG 0036. The support of the Materials and Manufacturing Directorate of the Air Force Research Laboratory is gratefully acknowledged.

10:24AM P32.00011 ABSTRACT WITHDRAWN —

10:36AM P32.00012 Electrically controlled g-factor and magnetism in conjugated metal-organic molecules 1, ZHI-GANG YU, SRI International — Conjugated metalorganic molecules have localized spins at the central transition-metal ions and mobile π-electrons in the surrounding ligands. Here we construct model Hamiltonians based on first-principles calculations to describe spins at the ions and π-electrons in the ligands. It is shown that the g-factor and magnetic susceptibility in such a molecule can be tuned to a great extent by an electrical voltage across one of the ligands. The underlying physics is that the voltage modifies the charge distribution of the ligand, which in turn changes the interplay of the ion’s spin-orbit coupling and the energy splitting among its orbital states. The capability of controlling the g-factor and magnetism at the molecular level has great implications in quantum information storage and processing.

1  This work was supported by the Office of Basic Energy Sciences, Department of Energy, under Grant No. DE-FG02-06ER46325.

10:48AM P32.00013 Magnetic-Field-Driven Ising Quantum Criticality of Two-Dimensional Square-Lattice Antiferromagnet Cr(dien)(O2)2.H2O — N. KAUR, G. PREAMPLUME, N. DALAL, Department of Chemistry, Florida State University, A. KUMAR, Department of Physics, Florida State University, Y. H. KIM, Y. TAKANO, Department of Physics, University of Florida, S. NELLUTLA, Y. J. JO, L. BALICAS, National High Magnetic Field Laboratory, Tallahassee, FL — We report on a systematic study of magnetically driven quantum phase transition in a new compound based on Cr(IV). The compound, Cr(dien)(O2)2.H2O, is a low-dimensional antiferromagnet with a Neel temperature TN of 2.55 K in zero field. We have used torque magnetometry, heat capacity and magnetocaloric-effect measurements down to 200 mK, to obtain a complete magnetic phase diagram. A detailed analysis of the dependence of TN on magnetic field using the power law TN ∝ (Hc−H)α yielded the critical exponent α = 2.01±0.02, with Hc = 12.392±0.003 T, indicating that this system behaves like a 3-d Ising magnet at low temperatures.

Wednesday, March 18, 2009 8:00AM - 10:48AM — Session P33 DCMP: Superconductivity: Electronic Structure II 403

8:00AM P33.00001 Universality of momentum-dependent charge-transfer excitations in the undoped cuprates measured by resonant inelastic X-ray scattering — GUILLAUME CHABOT-COUTURE, Stanford University, JASON HANCOK, Stanford University/SSRL, LI LU, PATRICK MANG, OWEN VAJK, Stanford University, DIEGO CASA, THOMAS GOG, Advanced Photon Source, ANL, MARTIN GREVEN, Stanford University/SSRL — From its conception, the study of charge-transfer excitations in the cuprates has driven the majority of resonant inelastic X-ray scattering (RIXS) research. Still, to this day, there exists more variation among published RIXS spectra and their interpretation than common ground. By carefully studying the momentum-dependent spectral weight of three of the most important undoped cuprates — La2CuO4, Nd2CuO4, and Sr2CuO3Cl2—we present evidence of universality of the observed charge-transfer excitations. To clarify and highlight this observation, we construct dispersion diagrams and study the incident energy dependence. Comparison to Hubbard model predictions suggests that the essence of this universality is captured already by one-band physics, while material dependence and cross-sectional effects only obfuscate this behavior.

8:12AM P33.00002 Momentum-Resolved Cu K-edge RIXS Spectra in the Insulating Parent Compounds of High Tc Superconductors — C-C. CHEN, B. MORITZ, Stanford University and SLAC, F. VERNAY, Paul Scherrer Institut, S. JOHNSTON, University of Waterloo and SLAC, J. HANCOK, G. CHABOT-COUTURE, M. GREVEN, Stanford University and SLAC, I. ELFIMOV, G. A. SAWATZKY, University of British Columbia, T. P. DEVEREAUX, Stanford University and SLAC — Resonant inelastic X-ray scattering (RIXS) has the ability to highlight various many-body excitations that can be characterized by photon momentum transfer and energy loss. Exact Diagonalization calculations on small clusters were carried out to investigate the nature of the excitations seen in RIXS spectra in the parent compounds of high Tc superconductors. The model many-body calculation includes electronic orbitals necessary to highlight Zhang-Rice singlets, charge transfer and d-d excitations, as well as states with significant apical character. The influence of different orbitals on the RIXS spectra is studied, and the character of the excitations in different regions of the Brillouin zone is determined as well.

8:24AM P33.00003 Momentum dependence of the electron-phonon coupling, phonon-induced pairing interaction, and self-energy effects in YBa2Cu3O7 within the local density approximation — ROLF HEID, KLAUS-PETER BOHNNEN, Forschungszentrum Karlsruhe, IFP, Germany, DIRK MANSKE, ROLAND ZEYHER, Max-Planck-Institut for Solid State Physics, Stuttgart, Germany — Using the local density approximation (LDA) and a realistic phonon spectrum we calculate the momentum and frequency dependence of the electron-phonon coupling in YBa2Cu3O7 and determine its consequences for the phonon-induced pairing interaction and for the electronic self-energy in the normal state. The phonon-induced interaction has a pronounced peak for large momentum transfers and the interband contributions between bonding and antibonding band are of the same magnitude as the intraband ones. The dimensionless coupling constant in the d-wave channel λd, relevant for superconductivity, is only 0.022, i.e., even about ten times smaller than the small value of the s-wave channel. For electronic states at the Fermi energy, the maximum in the real part of the phonon-induced self-energy at low frequencies is about a factor 5 too small compared to the experiment, resulting in a very small and smooth change in the slope of the electronic dispersion [1]. These findings suggest that phonons are not the important low-energy excitations, and cannot produce well-pronounced peaks in YBa2Cu3O7, at least, within LDA. [1] Heid, Bohnen, Zeyher,Manske, PRL 100, 137001 (2008).
8:36AM P33.00004 Electronic Properties of Rocksalt Copper Monoxide, PAUL MICHAEL GRANT, W2AGZ Technologies — Rocksalt copper monoxide, although not yet synthetically realized in bulk form, can be studied computationally as a proxy for the family of layered HTSC copper oxides. We report results for a series of tetragonal CuO rocksalt structures with c/a lattice parameter ratios ranging from 1.0 to 1.5, employing the plane-wave pseudopotential method with exchange-correlation LDA+U. As expected, we obtain a metallic state for U = 0 at all values of c/a given that the nominal valence electron configuration for Cu in copper monoxides is 3d10 yielding a partially occupied conduction band. However, completely unexpected was our finding similar nominal properties in rocksalt CuO for all physically plausible values of U (up to 10 eV) and c/a between 1.0 to approximately 1.2. Only for c/a > 1.2 do our calculations reveal the opening of a Mott-Hubbard charge-transfer gap. We interpret our results as supporting the original motivations of Bednorz and Mueller that high temperature superconductivity in the layered copper oxide perovskites may begin with their tendency to exhibit Jahn-Teller strong electron-phonon coupling.1


8:48AM P33.00005 Electronic Structure of Superconducting FeSe Studied by Photoemission Spectroscopy1, RIKIYA YOSHIDA, Okayama University, TAKANORI WAKITA, RLSS-Okayama University, JST-TRIP, HIROYUKI OKAZAKI, Okayama University, YOSHIKAZU MIZUGUCHI, University of Tsukuba, NIMS, SHUNSUKE TSUDA, NIMS, WPI-MANA-NIMS, JST-TRIP, YOSHIIHIKO TAKANO, NIMS, University of Tsukuba, JST-TRIP, HIROYUKI TAKEYA, KAZUTO HIRATA, NIMS, TAKAYUKI MURO, JASRI/SPRING-8, MARIO OKAWA, KYOKO ISHIZAKA, ISSP-The University of Tokyo, SHIK SHIN, ISSP-The University of Tokyo, RIKEN, HISATOMO HARIMA, Kobe University, JST-TRIP, MASAACKI HIRAI, YUJI MUROKA, TAKAYOSHI YOKOYA, RLSS-Okayama University, JST-TRIP — We have performed soft x-ray and ultrahigh-resolution laser photoemission measurements on tetragonal FeSe, which was recently identified as a superconductor. Energy dependent study of valence band is compared to band structure calculations and yields a reasonable assignment of partial densities of states. However, the sharp peak near the Fermi level slightly deviates from the calculated energy level, showing the importance of self-energy correction. We have also performed an ultrahigh-resolution laser photoemission experiment on FeSe and observed the suppression of intensity around the Fermi level upon cooling.

1Supported by MEXT, Japan

9:00AM P33.00006 Generic phase diagram of “electron-doped” T′ cuprates, M. NAITO, O. MATSUMOTO, A. UTSUKI, Tokyo University of Agriculture and Technology, A. TSUKADA, Stanford University, H. YAMAMOTO, NTT BRL., T. MANABE, AIST — The electronic phase diagram of cuprate superconductors is a key ingredient to understand the still unresolved mechanism of high-temperature superconductivity. A particular interesting question is the differences and similarities between the hole- and electron-doped sides. The phase diagram of hole-doped high-Tc cuprates has been well established, and shows a well-known “dome” shape with maximal superconductivity at a doping level of about 0.15. In contrast, the phase diagram of the electron-doped side is controversial. This is because the superconductivity in the T′ cuprates deteriorates seriously by the presence of impurity oxygen (Oimp) atoms, which have to be cleaned up in order to unveil the generic phase diagram of the T′-cuprates. We investigated the generic phase diagram of the electron doped superconductor, Nd2−xCexCuO4 using films prepared by metal organic decomposition. After careful oxygen reduction treatment to remove interstitial Oimp atoms, we found that the Tc increases monotonically from 24 K to 29 K with decreasing x from 0.15 to 0.00, demonstrating a quite different phase diagram from the previous bulk one. The implication of our results is discussed on the basis of tremendous influence of Oimp “impurities” on superconductivity and also magnetism in T′ cuprates.

9:12AM P33.00007 Band-theory description of hole localization and singlet polarons in doped cuprates, ALESSIO FILIPPETTI, DANilo PUGGINI, VINCENTMO FIORENTINI, CNR-INFM SLACS and University of Cagliari, CNR-INFM SLACS TEAM — We use an advanced ad-initio band theory (the pseudo-self interaction corrected local density approach, pSIC) to describe spin-compensated polarons (e.g. Zhang-Rice singlets (ZRS)) typical of low-dimensional doped cuprates. Despite their many-body nature, ZRS can be transparently interpreted via (and, in fact, constructed from) single-particle states, provided that band theory describes accurately enough their localization in the limit of vanishing band dispersion. We provide examples of polarons in real materials, specifically chain-like Ca2+1−yFe+yCu3O4 and the high-Tc superconductor (HTSC) Y1−x−3Ba2+xCu3O6+y. The former is the ideal prototype of doped one-dimensional cuprate with zig-zag Cu-O interactions. Studying the electronic and magnetic properties over the full range of possible doping, we identify several different polaron-dominated ground states and the attendant phase transitions. Furthermore, ZRS are key to the behavior of doped CuO2 units in HTSC. We show how their occurrence can dramatically affect the electronic properties (e.g. the Fermi surface) in underdoped Y1−x−3Ca2+xBa2−xCu3O6+y.

9:24AM P33.00008 Interplay of Ca and O doping in Y1−x−3Ca2+xBa2−xCu3O6+y studied by first-principles calculations, VINCENTMO FIORENTINI, ALESSIO FILIPPETTI, DANilo PUGGINI, CNR-INFM SLACS and University of Cagliari — Experiments reveal an impressive asymmetry in most aspects (involving e.g. magnetic, superconducting, or structural properties) of high-Tc superconductors upon cation or oxygen doping, respectively. A thorough understanding of this asymmetry cannot eschew a rigorous description of the fundamental mechanism ruling electronic and structural properties for each (x,y) doping combination. Here we present results obtained by the pseudo-self-interaction free density functional (pSIC) method, which is capable to describe metal-insulating transitions in several cuprate materials. We describe in detail the chemistry of the distinct insulating-metal transitions occurring in the CuO chains and in the CuO2 planes in the YBa2Cu3O6+y for y=0[0.5]. We then show that interactions with chains crucially affect the ability of Ca doping to inject holes in CuO2 planes. The dramatic effects of this double-doping interplay on the magnetic and superconducting properties of underdoped Y1−x−3Ca2+xBa2−xCu3O6+y cannot be understood by the disentangled action of the individual doping sources.

9:36AM P33.00009 Possible enhancements of AFM spin-fluctuations in high-Tc cuprates, THOMAS JARLBORG, DPNC, University of Geneva, CH-1211 Geneva 4, Switzerland — Ab-initio band calculations for high-Tc superconductors based of a free electron like band, show a strong interaction between anti-ferromagnetic (AFM) spin waves and periodic lattice distortions as for phonons, even though this type of spin-phonon coupling (SPC) is underestimated in calculations using the local density approximation. The SPC has a direct influence on the properties of the HTSC cuprates and it can explain many observations. The strongest effects are seen for modulated waves in the CuO bond direction, and a band gap is formed near the X,Y points, but unusual band dispersion (like “waterfalls”) might also be induced below the Fermi energy (EF) in the diagonal direction. The band results are used to propose different ways of increasing AFM spin-fluctuations locally, and to have a higher density-of-states (DOS) at EF. Static potential modulations, via periodic distribution of dopants or lattice distortions, can be tuned to increase the DOS. This opens for possibilities to enhance coupling for spin fluctuations (Δω) and superconductivity. The exchange enhancement is in general increased near a surface, which suggests a tendency towards static spin configurations. The sensitivity of the band results to corrections of the local density potential are discussed.
9:48AM P33.00010 Interband Transitions in La$_2-x$Sr$_x$CuO$_4$ observed by Resonant Inelastic X-Ray Scattering, D.S. ELLIS, JUNGHO KIM, H. ZHANG, University of Toronto, S. WAKIMOTO, JAERI, J.P. HILL, Brookhaven National Lab., Y. ANDO, S. KOMiya, CREIEL, D. CASA, T. GOc, Argonne National Lab., Y.-J. KIM, University of Toronto — Resonant inelastic x-ray scattering measures the energy and momentum dependence of electronic excitations, whose probabilities are resonantly enhanced, in this study, by utilizing hard x-rays at the Cu K-edge absorption energy. Three main features in the resonant inelastic x-ray scattering spectrum of La$_2-x$Sr$_x$CuO$_4$ were observed to develop as the doping $x$ increased from the underdoped to the overdoped region of the high-temperature superconductor phase diagram. Measured at the zone-boundary momentum transfer ($\sim 0$), the spectra consist of three main peaks: one peak below an isosbestic point at 2.2 eV which strengthens at high doping, and two broad peaks above - one at 3.3 eV increasing in energy and decreasing in intensity, and the other stationary at higher energy. Taking a cue from existing band structure calculations, these peaks are interpreted as the transitions between stationary bands of non-bonding Oxygen, a Zhang-Rice singlet type band at the Fermi level, and the upper Hubbard band. These transitions are also discussed in the context of existing angle-resolved photoemission data.

10:00AM P33.00011 Off gap interface reflectivity of electron waves in Fabry Perot resonators, ARITZ LEONARDO, P.M. ECHENIQUE, E. CHULKOV, F. SCHILLER, J.E. ORTEGA — The interface reflectivity in the MgW(110) metallic quantum well is from line shape analysis of high resolution photo emission. A quick reflectivity drop is found away from high band of the appropriate symmetry near Ef, such that the interface overcomes the bulk like quasi particle lifetime as the line broadening mechanism. A nearly free electron model for the W(110) substrate band structure demonstrates coherent wave function scattering is the relevant mechanism determines the interface reflectivity in the resonator.

10:12AM P33.00012 Quasiparticle dispersion anomaly induced by the spin excitation in electron-doped cuprates, TAO ZHOU, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston — It is proposed that the 50 – 70 meV dispersion anomaly (kink) in electron-doped cuprates revealed by recent angle-resolved photoemission spectroscopy experiments is caused by coupling with the spin fluctuation. We elaborate that the kink exists both along nodal and antinodal directions, and both in the superconducting and normal state. The renormalized effect for the density of states is also studied and the hump feature outside the superconducting coherent peak is established, consistent with recent scanning tunneling microscopy experiments.

10:24AM P33.00013 Weak flux pinning in the phase separated La$_2-x$Sr$_x$CuO$_{4+y}$ system, HASHINI MOHOTTALA, University of Hartford, BARRETT O. WELLS, JOSEPH I. BUDNICK, WILLIAM A. HINES, University of Connecticut — We have studied the magnetic characteristics of a series of super-oxygenated La$_2-x$Sr$_x$CuO$_{4+y}$ samples. According to our previous studies, these samples spontaneously phase separate to give an oxygen rich superconducting phase with a $T_c$ near 40 K and an oxygen poor magnetic phase that also orders near 40 K. All our samples showed a large reversibility in magnetization at different temperatures. Although the internal magnetic regions were expected to behave as pinning sites, our present study shows that they do not favor flux pinning. In terms of the matching principle between the defect and the coherence length, the regions that are larger than the coherence length cannot act as flux pinning centers. Thus our results imply that the magnetic regions are too large to act as pinning centers. Overall less flux pinning in the oxygen rich system also suggests that the separate superconducting regions in the system are more homogeneous.

This work was partially supported by the US-DOE through contract DE-FG02-00ER45801.


10:36AM P33.00014 Preparation of undoped superconducting T*-RE$_2$CuO$_4$ by MBE with ex-situ post-reduction, HIDEKI YAMAMOTO, NTT Basic Research Labs., OSAMU MATSUMOTO, MICHIO NAITO, Tokyo University of Agriculture and Technology — It has recently been revealed that the optimally-reduced end-member compounds T*-RE$_2$CuO$_4$ ($RE = Pr, Nd, Sm, Eu, Gd$) show superconductivity with $T_c$ over 30K [1] although they are commonly believed as Mott insulators. The superconducting specimens were produced by metal organic decomposition (MOD) with elaborated reduction procedures, where the advantage of thin-films, large surface-to-volume ratio, is fully utilized to achieve the optimal oxygen configuration. Their single-crystalline thin films prepared by UVH-based process may have a further advantage of providing a good opportunity to observe the superconducting order parameter highly in these materials using powerful but surface-sensitive probes such as ARPES and STM. With this motivation in mind, we grew 100-nm-thick T*-RE$_2$CuO$_4$ ($RE = Pr, Nd, Sm$) films on SrTiO$_3$ substrates by MBE. The as-grown films were semiconducting. However, with a post-reduction treatment in a tubular furnace, which is essentially identical to that for the MOD films, the MBE films became metallic and showed superconductivity at $\sim 30K$, indicating that the superconducting films are potentially obtainable through in-vacuo process by tuning up the reduction conditions. [1] O. Matsumoto et al., Physica C 468 (2008) 1148; M. Naito et al., J. Phys. Conf. Ser. 108 (2008) 012037.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P34 DCMP: Superconductivity: STM 404

8:00AM P34.00001 Heating Effects in Interlayer Tunneling Spectroscopy of Bi$_{2}$Sr$_{1-x}$Ca$_{x}$Cu$_{2}$O$_{y+\delta}$ as Inferred from Single Junction Methods, C. KURTER, Argonne National Lab., J.F. ZASADZINSKI, Illinois Institute of Technology, L. OZYUZER, Izmir Institute of Technology, D.G. HINKS, K.E. GRAY, Argonne National Laboratory, EMERGING MATERIALS GROUP TEAM, ILLINOIS INST. OF TECH. COLLABORATION, IZMIR INST. OF TECH. COLLABORATION — In order to study Joule-heating effects on small intrinsic Josephson junction (IJJ) stacks or mesas, we compare their current-voltage curves, I(V), with those of single junctions, both using Bi$_2$Sr$_{1-x}$Ca$_x$Cu$_2$O$_{y+\delta}$ (Ca-Bi2212) intercalated by HgBr$_2$. Even for small volume stacks with reduced dissipation by intercalation, there can be self-heating despite the absence of the commonly seen backbending of I(V). This conclusion is based on distinctive features of I(V) of intermediate size mesas which were absent in single junctions.

8:12AM P34.00002 Development of a novel variable temperature scanning tunneling microscope and discovery of spectral weight shift between two bands across Tc in underdoped Bi2212, JIHINHWAN LEE, K. FUJITA, C.K. KIM, A. SCHMIDT, LASSP, Cornell Univ., H. EISAKI, AIST, Japan, S. UCHIDA, Dept. of Physics, Univ. of Tokyo, Japan, J.C. DAVIS, LASSP, Cornell Univ. — We investigated the quasiparticle interference as a function of temperature for underdoped Bi2212 with Tc=42K, using the newly developed variable temperature STM. Due to increased $S/N$ and resolution, we could observe for the first time the dispersing octet peaks well above Tc. With novel high momentum resolution analysis we also found that each octet peak actually consists of two bands with distinct dispersions and observed clear spectral weight shift from one band, corresponding to the Bogoliubov quasiparticle whose dispersion depends sensitively on the temperature, to the other, with dispersion roughly following the normal state band structure with no significant temperature dependence, as we cross Tc from the superconducting state to the pseudogap state. This new discovery may shed new insight to our understanding of the pseudogap state of the underdoped cuprate superconductor.
8:24AM P34.00003 Imaging the Vortex Liquid State in Bi$_2$Sr$_2$CuO$_{8+\delta}$, T.L. WILLIAMS, M. ZECH, YI YIN, Harvard University, T. KONDO, Ames Laboratory, Iowa State University, T. TAKEUCHI, H. IKUTA, Nagoya University, J.E. HOFFMAN, Harvard University — We use a low temperature scanning tunneling microscope (STM) to study the vortex state of the high-$T_c$ superconductor Bi$_2$Sr$_2$CuO$_{8+\delta}$ in magnetic fields up to 9 T. At a temperature of 6 Kelvin, we find no localized vortices down to H = 0.25 T. However, the gap depth from the spatially averaged $d_{1/2}$ spectrum decreases with increasing magnetic field, which indicates a vortex liquid state. By tracking atomically resolved locations at different magnetic fields, we apply a normalization technique to remove inhomogeneities in the underlying density of states, revealing a more homogeneous superconducting state.

3We acknowledge support from NSF grant DMR-0508812 and AFOSR grant FA9550-05-1-0371.

8:36AM P34.00004 Coexistence of competing orders with two energy gaps in real and momentum space in the High $T_c$ Superconductor Bi$_2$Sr$_2$La$_x$CuO$_{8+\delta}$, JIJUA MA, Z.-H. PAN, F.C. NIESTEMSKI, M. NEUPANE, Y.-M. Xu, ZIQAING WANG, VIDYA MADHAVAN, Department of Physics, Boston College, M. ODA, M. IDO, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, N. MOMONO, Department of Materials Science and Engineering, Muroran Institute of Technology, Muroran 050-8585, Japan, M. ODA, M. IDO, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, NOKI MOMONO COLLABORATION, WPI ADVANCED INSTITUTE FOR MATERIALS RESEARCH, TOHOKU UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, TOHOKU UNIVERSITY COLLABORATION, INSTITUTE OF PHYSICS AND NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS OF CHINA COLLABORATION — We have performed scanning tunneling microscopy and angle-resolved photoemission spectroscopy on optimally doped and overdoped Bi$_2$Sr$_2$La$_x$CuO$_{8+\delta}$. We observe two distinct energy gaps that coexist both in real space and in the antinodal region of momentum space below $T_c$. We find that the small gap is associated with superconductivity. The large gap persists above $T_C$ and seems to be linked to observed charge order. We also find a strong correlation between these two gaps suggesting they are affected by similar physical processes.

8:48AM P34.00005 Coexistence of superconducting and pseudogap quasiparticles in underdoped Bi2212: Studies of STM/STS and ultra-fast optical spectroscopy, Y. H. LIU, T. KUROSAWA, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, Y. TODA, K. SHIMATAKE, Department of Applied Physics and Division of Innovative Research CRIS Hokkaido University, Sapporo 060-0810, Japan, N. MOMONO, Department of Materials Science and Engineering, Muroran Institute of Technology, Muroran 050-8585, Japan, M. ODA, M. IDO, Department of Physics, Hokkaido University, Sapporo 060-0810, Japan, NOKI MOMONO COLLABORATION, Y. TODA COLLABORATION — At present, the relationship between superconducting (SC) gap and pseudogap (PG) of cuprate superconductors is still under intense debate. Here, we present our recent results of the electronic structure and quasiparticle dynamics measured by STM/STS and ultra-fast optical spectroscopy on underdoped Bi2212 crystals, which provide direct evidence that SC and PG quasiparticles coexist below $T_c$. We will also discuss the origins of the periodic charge order and the nano-scale electronic inhomogeneity.

3}(Present address) Department of Physics and Astronomy, Ohio University, Athens, OH 45701

9:00AM P34.00006 Origin of electron-hole asymmetry in the scanning tunneling spectrum of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, A. Bansil, Northeastern U., JOUKO NIEMINEN, Tampere U. of Tech., Finland and Northeastern U., HSIN LIN, R. S. Markiewicz, Northeastern U. — We have developed a material specific theoretical framework for modelling scanning tunneling spectroscopy (STS) of high temperature superconducting materials in the normal as well as the superconducting state. Results for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ show clearly that the tunneling process strongly modifies the STS spectrum from the local density of states (LDOS) of the $d_{x^2-y^2}$ orbital of Cu. The dominant tunneling channel to the surface Bi involves the $d_{x^2-y^2}$ orbitals of the four neighboring Cu atoms. In accord with experimental observations, the computed spectrum displays a remarkable asymmetry between the processes of electron injection and extraction, which arises from contributions of $d_{x^2}$ and other orbitals to the tunneling current. Work supported in part by the USDOE.

9:12AM P34.00007 The Impact of an Oxygen Dopant in an ideal Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ Crystal, STEVE JOHNSTON, University of Waterloo, Waterloo, ON, Canada., FRANCOIS VERNAY, Paul Scherrer Institut, Villigen PSI, Switzerland, T. P. Devreux, SLAC National Lab, Stanford, Menlo Park, CA — Scanning tunneling microscopy studies have shown that local nanoscale pairing inhomogeneities are correlated with interstitial oxygen dopants in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Combining electrostatic and cluster calculations, we examine the impact of a dopant on the local Madelung and charge transfer energies, magnetic exchange $J$, Zhang-Rice mobility, and interactions with the lattice. It is found that electrostatic modifications locally increase the charge transfer energy and slightly suppresses $J$. It is further shown that coupling to c-axis phonons is strongly modified near the dopant. The combined effects yield broadened spectral features, reduced charge gap energies, and a sizable local increase of $J$ implying a strong local interplay between antiferromagnetism, polaron, and superconducting pairing.

9:24AM P34.00008 Tunneling Spectral Dip Feature in High Tc Cuprates: Experiment and Analysis, JOHN ZASADZINSKI, LIAM COFFEY, CHIAN KURTER, Illinois Institute of Technology, KEN GRAY, Argonne National Laboratory — A fully self-consistent Eliashberg analysis is presented to analyze the spectral dip feature observed in tunnel junctions on Bi2212. Methods include SIS break junctions, intrinsic Josephson junctions in mesas and SIN junctions from STM. This analysis is presented for a variety of doping levels and the resulting electron-boson spectral function and self-energy is compared with other spectroscopic probes. Evidence of spectral dip features in other high Tc cuprates is presented including Tl2212 to demonstrate the universality of the spectral dip and its relation to the mechanism of pairing.

9:36AM P34.00009 Phenomenological model of the bipartite electronic structure of Bi2Sr2CaCu2O8+d: Predicting bulk thermodynamic quantities from tunneling spectroscopy, J.W. ALLDREDGE, University of Colorado Boulder, K. FUJITA, Cornell University, JINHO LEE, Brookhaven National Laboratory, M. WANG, Cornell University, H. EISAKI, AIIST-Tsukuba, S. UCHIDA, University of Tokyo, P.J. HIRSCHFELD, University of Florida, J.C. DAVIS, Cornell University, K. MCELROY, University of Colorado Boulder — Using high quality local STM maps with corresponding quasiparticle interference data, we develop a complete phenomenological description of the density of states in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. This not only describes the local density of states but also consistently describes the spectral density of states derived from the QPI. The model consists of a d-wave gap structure at high energy. At low energies is has an additional higher harmonic term in the d-wave gap. Using this we capture not only the high energy gap signature but also the low energy features in the LDOS which accompany the termination of the QPI signal and this allows us to quantitatively measure the features across a wide series of dopings showing consistency between real and k-space. The use of this simple model allows us to successfully predict superfluid density, confirming that our model can successfully determine bulk physics from a local measurement.
there is a significant enhancement in the stability of vortices against thermal fluctuations. \[1\] Gorky Shaw, Shyam Mohan, Jaivardhan Sinha and S. S. Banerjee* the blind holes pins which creates a barrier against vortex redistribution inside the sample. We propose that this barrier leads to a phase separation creating significant magnetic field sweep rate dependent metastable magnetization response \[1\]. Our results are explained on the basis of a unique collective action of 1stitial vortices as bosonic modes. We investigate these modes with increasing oxygen reduction which represents the third dimension in the electron-doped superconducting crystal with otherwise C4 rotational symmetry, stripe orientations in the presence of quenched disorder map to the random field Ising model. While the low temperature scanning tunneling microscope (STM). The effect of individual atomic impurities on the superconducting state has been studied. Tunneling spectroscopy at 0.4 K reveals clear spectroscopic signature of the magnetic impurities at atomic scale. We find that Co is in the weak scattering limit and the tunneling spectra are homogeneous on the sample surface with sharp coherent superconducting peaks. Mn instead acts as a strong scatter destroying superconductivity at atomic scale, even when the number of impurities is limited to just a few in a correlation volume. The effect of intercalation on the charge density waves will be discussed as well. This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory (‘Argonne’). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357.

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1 NSF Grant DMR-0405088.
2 Currently at Physics Dept., Harvard, Cambridge, MA

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10:00AM P34.00011 STM studies of Co$_x$NbSe$_2$ and Mn$_x$NbSe$_2$ MARIA JAVARONE, GORAN KARAPETROV, Materials Science Division, Argonne National Laboratory, ROBERTO DI CAPUA, Dipartimento S. pe. S., Universita degli Studi del Molise, Campobasso I-86100, Italy, ALEX KOSHELEV, DANIEL ROSENMANN, Materials Science Division, Argonne National Laboratory, TERUKAZU NISHIZAKI, NORIO KOBAYASHI, Institute for Materials Research, Tohoku University, Japan — The effect of the intercalation of Co and Mn into the 2H phase transition-metal dichalcogenide NbSe$_2$ has been investigated with a low temperature scanning tunneling microscope (STM). The effect of individual atomic impurities on the superconducting state has been studied. Tunneling spectroscopy at 0.4 K reveals clear spectroscopic signature of the magnetic impurities at atomic scale. We find that Co is in the weak scattering limit and the tunneling spectra are homogeneous on the sample surface with sharp coherent superconducting peaks. Mn instead acts as a strong scatter destroying superconductivity at atomic scale, even when the number of impurities is limited to just a few in a correlation volume. The effect of intercalation on the charge density waves will be discussed as well. This work was supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory (‘Argonne’). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357.

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10:12AM P34.00012 Observation of vortices and hidden pseudogap from scanning tunneling spectroscopic (STS) studies of electron-doped cuprate superconductor La$_{1.85}$Sr$_{0.15}$CuO$_2$ (La-112) M.L. TEGUE, A.D. BEYER, N.-C. YEH, Phys. Dept, Caltech, Pasadena, CA, USA, S.-I. LEE, Phys. Dept Sogang U, Seoul, Korea — We present STS studies on the electron-doped cuprate superconductor La-112 as a function of magnetic field (H). The spatially resolved spectra manifest vortices, and the average vortex lattice constant scales consistently with Abrikosov’s theory. A hidden pseudogap ($V_{CO}$) smaller than the superconducting gap ($\Delta_{SC}$) is revealed inside the vortex core, and the core radius is comparable to the superconducting coherence length $\xi_{ab} = 4.86 \text{ nm}$. Analysis of the energy histograms reveals that $\Delta_{eff}$, where $\Delta_{eff}= [(\Delta_{SC})^2+(V_{CO})^2]^{1/2}$, shifts downward with increasing H from $\Delta_{eff}=122 \pm 0.8 \text{ meV}$ at H = 0 to a base value of $V_{CO}=8.5 \pm 0.6 \text{ meV}$ at H > 0. This finding differs from the behavior of conventional superconductors where the vortex-state spectral weight would shift continuously to lower energies with increasing H and show peaks at zero energy due to suppression of $\Delta_{SC}$ inside vortices. Finally, Fourier transformation of the vortex-state tunneling spectra will be reported and compared with results from other cuprates. Ref.: Teague et al., arxiv:0809.0541. Work supported by NSF Grant DMR-0405088.

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10:24AM P34.00013 Noise Predictions for STM in Systems with Local Electronic Nematic Order, ERICA CARLSON, Purdue University, YEN LEE LOH, Ohio State University, KARIN DAHMEN, University of Illinois at Urbana-Champaign — We propose that thermal noise in local stripe orientation should be readily detectable via STM on systems in which local stripe orientations are strongly affected by quenched disorder. Stripes, a unidirectional, nanoscale modulation of electronic charge, are strongly affected by quenched disorder in two-dimensional and quasi-two-dimensional systems. While stripe orientations tend to lock to major lattice directions, dopant disorder locally breaks rotational symmetry. In a host crystal with otherwise C4 rotational symmetry, stripe orientations in the presence of quenched disorder map to the random field Ising model. While the low temperature state of such a system is generally a stripe glass in two dimensional or strongly layered systems, as the temperature is raised, stripe orientational fluctuations become more prevalent. We propose that these thermally excited fluctuations should be readily detectable in scanning tunneling spectroscopy as telegraph noise in the high voltage part of the local I(V) curves. We predict the spatial, temporal, and thermal evolution of such noise, including the circumstances under which such noise is most likely to be observed. In addition, we propose an in-situ test for assessing whether such noise is due to correlated fluctuations rather than independent switches.

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10:36AM P34.00014 STM Study of Bosonic Modes in the Cuprate Superconductor Pr$_{0.88}$LaCe$_{0.12}$CuO$_4$, VIDYA MADHAVAN, FRANCIS NIESTEMSKI, Boston College Dept. of Physics, SHILIANG LI, University of Tennessee, PENGCHENG DAI, University of Tennessee & ORNL — We use a low temperature (4 K) ultra-high vacuum scanning tunneling microscope (STM) to investigate the electron-doped high temperature superconductor Pr$_{0.88}$LaCe$_{0.12}$CuO$_4$ (PLCCO). We examine the superconducting gap and the satellite features identified as bosonic modes. We investigate these modes with increasing oxygen reduction which represents the third dimension in the electron-doped superconducting phase diagram. We relate our findings to neutron scattering results performed on the same sample.

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10:48AM P34.00015 Collective action of nanopatterned pins: barrier towards creating inter-stitial vortices*, GORKY SHAW, SHYAM MOHAN, JAIvardhan SINHA, SATYAJIT BANERJEE, Department of Physics, Indian Institute of Technology, Kanpur-208016, U. P., India — We show that by nano-patterning a superconductor (NbSe$_2$ singlecrystal) with an array of blind holes produces significant magnetic field sweep rate dependent metastable magnetization response.[1]. Our results are explained on the basis of a unique collective action of the blind holes pins which creates a barrier against vortex redistribution inside the sample. We propose that this barrier leads to a phase separation creating distinct population of vortices viz., those pinned on blind holes and those confined in the interstitials between the holes [1]. We find that due to the barrier, there is a significant enhancement in the stability of vortices against thermal fluctuations. [1] Gorky Shaw, Shyam Mohan, Jaivardhan Sinha and S. S. Banerjee* (submitted; xxx.lanl.gov/abs/0811.1256) *satyajit@itk.ac.in

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3 SSB acknowledges funding support from CSIR and DST, India.
8:00 AM P35.00001 Low-temperature thermal transport properties of BaNi$_2$As$_2$. NOBUYUKI KURITA, FILIP RONNING, YOSHIFUMI TOKIWA, ERIC D. BAUER, Los Alamos National Laboratory, ALASKA SUBEDI, Oak Ridge National Laboratory and University of Tennessee, DAVID J. SINGH, Oak Ridge National Laboratory, JOE D. THOMPSON, ROMAN MOYSHOVICH, Los Alamos National Laboratory — Low-temperature specific heat $C(T)$ and thermal conductivity $\kappa(T)$ measurements under magnetic field have been performed on a recently discovered Ni-based superconductor BaNi$_2$As$_2$ ($T_c \approx 0.7 K$). In zero field, $\kappa(T)$ shows $T^4$-linear behavior in the normal state and exhibits a BCS-like exponential decrease below $T_c$. The field dependence of the residual thermal conductivity extrapolated to zero temperature is indicative of a fully gapped superconductor. This conclusion is supported by the analysis of $C(T)$ data, which are well fit based on the BCS theory.

8:12 AM P35.00002 Anisotropy of electronic transport in the iron-pnictide superconductor Ba(Fe,Co)$_2$As$_2$. MAKARIY A. TANATAR, Ames Laboratory, N. NI, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, C. MARTIN, Ames Laboratory, R.T. GORDON, H. KIM, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, V.G. KOGAN, G.D. SAMOLYUK, S.L. BUD'KO, Ames Laboratory, P.C. CANFIELD, R. PROZOROV, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — The anisotropy of electrical resistivity in the iron pnictide superconductor Ba(Fe,Co)$_2$As$_2$ has been studied using the Montgomery technique and direct transport measurements in single crystals cut along principal directions of the conductivity tensor (tetragonal c-axis and a-direction perpendicular to it). A good quantitative agreement is found between two sets of data, with a $\rho_c/\rho_\|$ anisotropy of 5 ± 1 just above the superconducting transition temperature. This is in very good agreement with expectations based on the anisotropy of the critical fields, suggestive of orbital limiting of superconductivity at $T_c$.

8:24 AM P35.00003 C-axis transport of pnictide single crystals. YURI KOVAL, PAUL MUELLER, University Erlangen-Nuernberg, Germany, GUENTER BEHR, BERND BUECHNER, IFW Dresden, Germany — Mesta-type structures of ~1 $\mu$m$^2$ area were fabricated on the (ab) plane of small LaO$_{0.8}$F$_{0.2}$As FeAs single crystals. Resistance vs. temperature measurements showed a metallic behavior with a residual resistance ratio higher than 10. Both magnetic susceptibility and transport measurements showed the same value for the critical temperature, i.e. $\sim$80K. Current-voltage characteristics are typical for overdamped Josephson junctions with a critical current density of $\sim$10$^7$ A/cm$^2$. Moreover, the critical current vs. temperature dependence follows the Ambegaoker-Baratoff relation for the maximum dc Josephson current. One possible explanation could be that we have observed an intrinsic Josephson effect in $c$-direction. This is supported by recent measurements of radiation emission between 11 and 12 GHz. Finally, we discuss current injection effects on Josephson critical current and $T_c$.

8:36 AM P35.00004 Thermoelectric Power of RO$_{1-y}$Fe$_y$As. FENG CHEN, KALYAN SASMAL, MELISSA GOOCH, FENGYAN WEI, BERND LORENZ, YUYI XUE, C.W. CHU, Dept. of Physics and Texas Center for Superconductivity, University of Houston, Houston, TX 77004-5002, BING LV, ZHONGJIA TANG, ARNOLD GULOY, Dept. of Chemistry, University of Houston, Houston, TX 77204 — The thermoelectric power $S(T)$ has been measured on the RO$_{1-y}$Fe$_y$As samples with $0 \leq x \leq 0.3$ and $0 \leq y \leq 0.5$ and with the rare earth R = La, Ce, Sm and Pr. Together with Hall and lattice parameter studies, systematic x-dependence is observed, although rather weak for samples with $x > 0$ and $y = 0$. The $S(T)$ of the undoped samples with $x = y = 0$, however, appears to have rather different shape and amplitude. By comparing with the resistivity drop around 150 K, the change seems to be associated with the spin/lattice instability previously proposed.

8:48 AM P35.00005 A novel non-Fermi-liquid state in the iron-pnictide FeCrAs. WENLONG WU, ALIX MCCOLLAM, University of Toronto, IAN SWAINSON, National Research Council of Canada, PATRICK ROURKE, University of Toronto, DENIS RANCOURT, University of Ottawa, STEPHEN JULIAN, University of Toronto — We report transport and thermodynamic properties of stoichiometric single crystals of the hexagonal iron-pnictide FeCrAs. The in-plane resistivity shows an unusual “non-metallic” dependence on temperature $T$, rising discontinuously with decreasing $T$ from $\sim$ 800 K to below 100 mK. The $c$-axis resistivity is similar, except for a sharp drop upon entry into an antiferromagnetic state at $T_N \approx 125$ K. Below 10 K the resistivity follows a non-Fermi-liquid power law, $\rho(T) \sim T^\alpha$ with $\alpha < 1$. The specific heat, on the other hand, shows typical Fermi liquid behavior with a linear temperature dependence and a large Sommerfeld coefficient, $\gamma \sim 30$ mJ/mol K$^2$. The magnetic susceptibility does not follow Curie-Weiss law and it is rather weakly temperature dependent at low temperature. The high temperature properties of FeCrAs are reminiscent of those of the parent compounds of the new layered iron-pnictide superconductors, however the $T \rightarrow 0$ K properties suggest a new class of non-Fermi liquid. This low temperature state has some features expected of a fractionalized electron system, in which conduction electrons break up into a charge carrying part that scatters anomalously and a spin part that has the thermodynamic properties of a Fermi liquid.

9:00 AM P35.00006 Large quasiparticle thermal Hall conductivity in the superconductor Ba$_{1-x}$K$_x$Fe$_2$As$_2$. JOSEPH CHECKELESKY, LU LI, Princeton University, G.F. CHEN, J.L. LUO, N.L. WANG, Inst. of Physics, Beijing, China, N.P. ONG, Princeton University — We have measured the thermal conductivity $\kappa_{xy}$ and thermal Hall conductivity $\kappa_{xy}$ in single-crystal Ba$_{1-x}$K$_x$Fe$_2$As$_2$. Below the superconducting transition temperature $T_c (\sim 30 K)$, we observe a large peak in the weak-field $\kappa_{xy}$. A corresponding peak in the zero-field thermal conductivity $\kappa_{xy}$ is also observed. Together, these imply the existence of a large population of hole-like quasiparticles below $T_c$. In magnetic fields $H$ approaching 35 T, the peaks in $\kappa_{xy}$ are strongly suppressed. A fit of the $\kappa_{xy}$ vs. $H$ curves shows that the data are consistent with the scattering of long-lived quasiparticles by vortices. Using these fits, we have extracted estimates of the quasiparticle mean-free-path, and separated the zero-field electronic and phononic terms $\kappa_e$ and $\kappa_p$, respectively. We discuss the origin of the large quasiparticle population in terms a strongly anisotropic gap parameter or a gap with nodes.

9:12 AM P35.00007 Fe pnictides in high magnetic fields. FEDOR BALAKIREV, Los Alamos National Laboratory — High magnetic fields provide invaluable tool in probing such complex and phase-rich materials as novel pnictide superconductors, where upper critical field estimates surpass 100 Tesla for some of the compositions. We have investigated a number of tertiary and quaternary iron pnictides in pulsed magnetic fields exceeding 60 T and will present the latest data on their superconducting and normal state properties at high fields. We probe the importance of reduced dimensionality for high temperature superconductivity across different families of pnictides, where we find contrasting behavior between 122 and 1111 compounds. We find clear signature of the Fermi surface reconstruction in magnetotransport properties of the field-induced normal state, which coincides with reported structural and magnetic phase transitions.

1Supported by NSF grant DMR 0213706 and DMR 0819860. Research at IOP is supported by NSFC, 973 project of MOST and CAS of China. High-field experiments were performed at the National High Magnetic Field Laboratory, Tallahassee.

2The work at the NHMFL was supported by the NSF, DOE, and by the State of Florida.
9:48AM P35.00008 Spin density wave instability and pseudogap formation in EuFe2As2. JONG HOON SHIN, SOON JAE MOON, Seoul National University, JU-YOUNG KIM, Gwangju Institute of Science and Technology, SEUNG HYUN KIM, WOO SEOK CHOI, BYUNG CHUL JEON, Seoul National University, YUN SANG LEE, Soongsil University, BEONG KI CHO, Gwangju Institute of Science and Technology, KHEE KIM KIM, TAE WON NOH, Seoul National University — Recently, iron arsenide superconductors have aroused great amount of interest. In these compounds, by doping electron or hole, the superconductivity arises with the suppression of spin density wave (SDW) order. The close relation between the CDW and SDW instability suggests that the magnetic fluctuation might play an important role. Therefore, it is imperative to study the magnetic ground state of the parent compounds to understand the mechanism of the superconductivity. We investigated optical conductivity spectra of EuFe2As2 single crystals, which showed SDW order below about 190 K. Across the transition temperature, the optical spectral weight transferred from low energy (below 900 cm-1) to higher energy (above 900 cm-1), forming a pseudogap. In the SDW phase, the sharp Drude-like response still remained. Our results indicate that the SDW formation induce the partial gap opening in the Fermi surface of EuFe2As2.

10:00AM P35.00009 Electronic anisotropy from magneto-transport near Tc in SmFeAs(O1−xF2x) and (Ba,Rb)Fe2As2 single crystals. PHILIP MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, KARSTEN KUNZE, Electron Microscopy ETH Zurich, Switzerland, ZBIGNIEW BUKOWSKI, NIKOLAI ZHIGADLO, JANKUSZ KARPINSKI, High Pressure Materials Synthesis, ETH Zurich, ZHANG HU, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We derived thermally activated flux flow (TAFF) activation energies EF (H) and the upper critical fields HC2(T) parallel to the c-axis and in the Lorentz-force free configuration (H // ab || j) of SmFeAs(O1−xF2x) and (Ba,Rb)Fe2As2 single crystals from resistance measurements and compare them to the ones reported for other REFeAs(O) compounds. A perfectly rectangular rod (67x11x4 µm), aligned with the crystal axes, was cut from a larger SmFeAs(O1−xF2x) single crystal (~200 µm) by a Focused Ion Beam (FIB) which allowed us to precisely control its geometric factor L/A = 0.89 1/µm. The FIB was also used to deposit 4 Pt contacts. We found a slope of Hc2,50% (T), parallel to the c-axis, of 1.9 T/K for SmFeAs(O1−xF2x) and 3.7 T/K for (Ba,Rb)Fe2As2 near Tc. The electronic anisotropy, derived from magneto-transport, is significantly larger in the REFeAs(O) crystals than in (Ba,Rb)Fe2As2.

10:12AM P35.00010 Quantum critical regime in the phase diagram of KxSr1−xFe2As2. BERND LORENZ, MELISSA GOOCH, TCSUH and Dept. of Physics, University of Houston, BING LV, ARNOLD M. GULOY, TCSUH and Dept. of Chemistry, University of Houston, CHING-WU CHU1, TCSUH and Dept. of Physics, University of Houston — The electrical and thermoelectric properties of KxSr1−xFe2As2 are investigated. While the temperature dependence of the resistivity of SrFe2As2 (x=0) and KFe2As2 (x=1) is strongly nonlinear over a large temperature range it becomes surprisingly linear for x close to xcr = 0.4 above the superconducting transition. This apparent deviation from the Fermi liquid behavior is similar to the high-Tc cuprate superconductors and may indicate the existence of a quantum critical regime above the superconducting dome. We show that the temperature dependence of the thermoelectric power S follows a logarithmic scaling, S/T = const.·log(T) at the critical value xcr. The experimental results are consistent with a Ginzburg-Landau model for FeAs compounds predicting quantum critical scaling with a dynamical exponent d+z=4.

1This work is supported by the T.L.L. Temple Foundation, the J.J. and R. Moores Endowment, the State of Texas through TCSUH, the DoE, the NSF, and the R. A. Welch Foundation.
2Also at: LBNL Berkeley and HKUST Hong Kong

10:24AM P35.00011 Low temperature thermal conductivity of single crystal Ba1−xKxFe2As2. J.-P. REID1, M.A. TANATAR2, X. LUO1, N. DOIRON-LEYRAUD1, N. NI1, S.L. BUD’KO2,3, P.C. CANFIELD2,3, H. LUP4, Z. WANG5, H.H. WEN4, R. PROZOROV2,3, LOUIS TAILLEFER1, DÉPARTEMENT DE PHYSIQUE, UNIVERSITÉ DE SHERBROOKE, QUÉBEC, CANADA TEAM, 2AMES LABORATORY, AMES, IOWA, USA COLLABORATION, 3DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY, AMES, IOWA, USA Collaboration, 4NATIONAL LABORATORY FOR SUPERCONDUCTIVITY, CHINESE ACADEMY OF SCIENCES, CHINA COLLABORATION — Novel iron-arsenic based superconductors with Tc up to 34 K for KxFe2As2 with x=0.25. We find no residual linear term in zero magnetic field and can therefore exclude a superconducting gap with a line of nodes.

10:36AM P35.00012 Effects of Co substitution on thermodynamic and transport properties and anisotropic Hc2 in Ba(Fe1−xCo2x)2As2. Y. NI, M. E. TILLMAN, J.-Q. YAN, A. KRACHER, S. L. BUD’KO, P. C. CANFIELD, Ames Lab / Iowa State University, S. T. HANNAHS, NHMFL, Tallahassee — Single crystal samples of Ba(Fe1−xCo2x)2As2, x<0.12, have been characterized by microscopic, thermodynamic and transport measurements. With increasing Co concentration, the features of the structural and magnetic transitions are suppressed at a rate of roughly 15K per percent of Co. Superconductivity is stabilized at low temperatures for 0.038 ≤ x ≤ 0.08 and up through our highest doping level of x = 0.114. The superconducting region has a dome like appearance with maximum Tc values (~23 K) found near x~0.07. The T−x phase diagram shows that either the existence of superconductivity in both the tetragonal and the orthorhombic (AFM) phase or there is a structural phase separation. Anisotropic Hc2 data clearly show that the superconductivity which occurs in samples that show features associated with the transition to the low temperature orthorhombic state is 50% smaller than that found in samples that remain in the tetragonal phase. These data show that the superconductivity is sensitive to the suppression of the higher temperature phase transition.

1Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.
9:30AM P36.00002 Physics Q & A — APS’s latest publication, Physics (http://physics.aps.org/), highlights exceptional papers from the Physical Review Journals. Each week, editors from the journals choose papers that merit this treatment, aided by referee comments and internal discussion. Physics features expert commentaries written by active researchers who are asked to explain the results to physicists in other subfields. These commissioned articles are edited for clarity and readability across fields and are accompanied by explanatory illustrations. Please join us for a session that will include a brief presentation by the editors of Physics followed by a Q and A.

Wednesday, March 18, 2009 8:00AM - 10:36AM — Session P37 DCP: Focus Session: Structure and Dynamics of Interfacial Water I

8:00AM P37.00001 Electron Solvation Dynamics at D$_2$O Ice and Na/D$_2$O/Metal Interfaces. MARTIN WOLF, Free University Berlin and Fritz-Haber-Institut, Berlin, Germany — Electron transfer (ET) across interfaces is of vital importance in different areas of physics, chemistry and biology. Using time-resolved two-photon-photoemission spectroscopy we have studied the ultrafast dynamics of interfacial ET and solvation processes in amorphous and crystalline D$_2$O layers on single crystal metal substrates and the influence of coadsorbed Na ions. In these experiments, photoionization of electrons from the metal into the adsorbate conduction band is followed by ultrafast localization and solvation of the excess electrons. The subsequent energetic stabilization of these solvated electrons due to nuclear rearrangements of the polar molecular environment is accompanied by an increasing degree of localization. The observed ET rates strongly depend on the local structure of the ice. In crystalline D$_2$O layers we monitor the stabilization of trapped electrons at the ice vacuum interface continuously from femtoseconds up to minutes. This behavior observed for crystalline ice is fundamentally different from amorphous D$_2$O layers where the excess electrons have a much lower survival probability, which lifetimes of the order of 100 fs, which extend to several 10 ps if Na ions are coadsorbed at the ice surface.

8:36AM P37.00002 Electron dynamics and intermolecular energy transfer in aqueous solutions studied by X-ray electron spectroscopy. BERND WINTER, BESSY, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany — X-ray photoelectron spectroscopy measurements from a vacuum liquid microjet are performed to investigate the electronic structure of aqueous solutions. Here, focus is on the excited-state dynamics of chloride and hydroxide anions in water, following core-level excitation. A series of Cl$^-$(aq) charge-transfer-to-solvent (CTTS) states, and their ultrafast relaxation, on the time scale of the core hole, is identified from the occurrence of spectator Auger decay. Resonant oxygen 1s excitation of aqueous hydroxide, in contrast, leads to non-local decay, involving energy transfer into a neighboring water molecule. This channel is argued to arise from the weak hydrogen donor bond of OH$^-$(aq), and thus identifies a special transient hydration configuration, which can explain hydroxide’s unusual and fast transport in water. Analogous measurements from pure water point to a similar relaxation channel, which is concluded from a strong isotope effect. The characteristic resonant spectral features are considerably stronger for H$_2$O(aq) than for D$_2$O(aq). As for OH$^-$(aq) the results can be understood in terms of energy transfer from the excited water molecule to a neighbor water molecule.

9:12AM P37.00003 Electrons tunneling through fluctuating water and proteins. DAVID BERATAN, Duke University — We have analyzed the characteristics of electron tunneling through thermally-fluctuating water and protein media [1]. A metric is defined that indicates when the tunneling propagation is well described by the average donor-acceptor tunneling interaction, as opposed to being dominated by medium fluctuations. Indeed, there is a transition distance that establishes a change in mechanism, and this distance is different for water-mediated compared to protein-mediated tunneling. Even in the fluctuation-dominated regime, we find that the three-dimensional protein fold controls the tunneling interactions. We also find that pairs of proteins in near contact may establish particularly strong water-mediated tunneling routes [2].


10:00AM P37.00005 X-ray studies of the Density Depletion at Hydrophobic Water-Solid Interfaces. MARKUS MEZGER, Lawrence Berkeley National Lab, Berkeley, HARALD REICHERT, HEIKO SCHRODER, JOHN OKASINSKI, ROLAND ROTH, HELMUT DOSCH, Max Planck Institute for Metals Research, Stuttgart, Germany, SEBASTIAN SCHODER, VEJO HONKIMAKI, European Synchrotron Radiation Facility, Grenoble, France, JOHN RALSTON, Ian Wark Research Institute, Mawson Lakes, Australia — Deeply buried hydrophobic solid-water interfaces were probed with high-energy x-ray reflectivity. The experimental data provide clear evidence for a thin density depletion with an integrated deficit corresponding to approximately 40% of a water monolayer extending over a maximum of two molecular layers. In addition, measurements on the influence of gases (Ar, Xe, Kr, N$_2$, O$_2$, CO, CO$_2$) dissolved in the water have been performed. No effect on the hydrophobic water gap was found. The presence of nanobubbles at the interface could also be excluded. By comparing the experimental results with an generic DFT model we can give a quantitative estimation for different contributions to the observed gap size.

The persistent demand for cheaper and high efficient catalysts in industrial chemical syntheses, such as ammonia, and in novel energy applications, hydrogen generation and purification in fuel cells motivated us to study the fundamental interaction involved in water-Cu system, with an intention to examine Cu as a possible competitive candidate for cheaper catalysts. Water structure and dissociation kinetics on a model open metal surface: Cu (110), have been investigated in detail based on first-principles electronic structure calculations. We revealed that in both monomer and overlayer forms, water adsorbs molecularly, with a high tendency for diffusion and/or desorption rather than dissociation on clean surfaces at low temperature. With the increase of the water coverage on the Cu (110) surface, the H-bond pattern lowers the dissociation barrier efficiently. More importantly, if the water molecule is dissociated, the hydrogen atoms can diffuse freely along the [110] direction, which is very useful in the hydrogen collection. In addition, we extended to study water on other noble metal (110) surfaces. The result confirms that Cu (110) is the borderline between intact and dissociative adsorption, differing in energy by only 0.08 eV. This may lead to promising applications in hydrogen generation and fuel cells.

8:00AM P38.00001 Nanoscale Architectures for Energy Applications¹, STANISLAUS WONG, Department of Chemistry at the State University of New York at Stony Brook — In my group, we have developed a number of different potential architecture systems for gaining insights into energy storage and photovoltaics. In one manifestation of our efforts, generating a heterojunction comprising nanotubes and nanocrystals, to create a sharp junction interface, whose properties are inherently manipulable, tailorable, and, hence, predictable. For example, the electrical resistance of nanotube-nanoparticle networks is dependent on the nanoscale junctions that exist between these constituent nanomaterials as well as on microscale and macroscale connectivity. Thus, rational design of these nanomaterials is critical to a fundamental understanding of charge transport in single molecules and the determination of their conductance. Results on these systems can therefore be used to increase understanding of intrinsic factors affecting carrier mobility, such as electronic structure, carrier trapping, and delocalization. In a second manifestation, three-dimensional, dendritic micron- scale spheres of alkali metal hydrogen titanate 1D nanostructures (i.e.: nanowires and nanotubes) have been generated using a modified hydrothermal technique in the presence of hydrogen peroxide and an alkali metal hydroxide solution. Sea-urchin-like assemblies of these 1D nanostructures have been transformed into their hydrogen titanate nanotube analogues by neutralization as well as into their corresponding semiconducting, anatase titanate nanostructured counterparts through a moderate high-temperature annealing dehydration process without destroying the 3D hierarchical structural motif. The as-prepared hollow spheres of titanate and titanita 1D nanostructures have overall diameters, ranging from 0.8 μm to 1.2 μm, while the interior of these aggregates are vacuous with a diameter range of 100 to 200 nm. We have demonstrated that these assemblies are useful for example as active photocatalysts for the degradation of synthetic Procion Red dye under UV light illumination. In a third set of experiments, a size- and shape-dependent morphological transformation was demonstrated during the hydrothermal soft chemical transformation, in neutral solution, of titanate nanostructures into their anatase titanita counterparts. Our results indicate that as-synthesized titanita nanostructures possessed higher photocatalytic activity than the commercial titanita precursors from whence they were derived.

¹National Science Foundation and Department of Energy.

9:12AM P38.00003 Electronic Dynamics in Nanocrystalline TiO₂ and ZnO Measured by Terahertz Spectroscopy, CHARLES SCHMUTTENMAER, Yale Univery, Department of Chemistry, JASON BAXTER, Dept. of Chemical and Biological Engineering — Understanding the microscopic details of carrier transport in nanocrystalline colloidal thin films is required for complete understanding of a variety of photochemical and photocurrent-driven cells utilizing interpenetrating networks. Measuring the photoconductivity in these materials, however, is a challenging problem because of the inherent difficulty of attaching wires to nanometer-sized objects. Furthermore, picosecond carrier dynamics play an important role in efficient charge separation and transport, but the low temporal resolution of traditional methods used to determine their photodetectivity precludes their use in studying sub-ps to ps dynamics. This talk will present recent advances utilizing THz spectroscopy to investigate and elucidate the microscopic behavior of carrier dynamics within the context of materials for energy applications such as dye-sensitized solar cells and solar-driven cells for catalytic and photoelectrochemical applications.

9:24AM P38.00004 Theoretical investigation of the high energy excitations in silicon nanocrystals, ADAM GALI, MARTON VOROS, Budapest University of Technology and Economics, DARIO ROCCA, GERELY ZSOMBOR, GIULIA GALLI, UC Davis — Recently, efficient multi-exciton generation (MEG) has been reported for several nanoclusters including silicon nanocrystals (SiNC). However, the existence of MEG has been disputed in the literature. The reported bi-exciton states in SiNC involve high energy empty states of SiNC. These states are expected to be very delocalized, and thus easily modified by the environment surrounding the SiNCs. In addition, the SiNCs are fabricated in a solution that usually contains CnHm molecules, e.g. hexane, that may bind to the surface of SiNCs, and modify their absorption spectrum. We have studied the absorption spectra of hydrogenated SiNCs by first principles calculations. The geometry was optimized within density functional theory (DFT), while absorption spectra were determined by time-dependent DFT. The effect of the environment on the SiNC was modeled by i) varying the distance between the nanoparticles ii) allowing for surface reconstruction and iii) monitoring the effect of absorption of CnHm groups on absorption spectra. We found that the high energy spectrum of SiNCs strongly depends on the environment. Our findings indicate that taking into account effects of surface states and SiNCs concentration in solution is crucial, in order to understanding multi exciton generation.

Wednesday, March 18, 2009 8:00AM - 11:00AM — Session P38 DCP: Focus Session: Nanomaterials for Energy Applications — 1
9:36AM P38.00005 Fast exciton relaxation and multiple exciton generation (MEG) in semiconductor nanocrystals: the role of defects. CHRISTOPHE DELEURIE, GUY ALLAN, IEMN-ISEN — Recent works have concluded that a single high-energy photon could generate multiple excitons in semiconductor nanocrystals but these results are debated and are not well understood theoretically. More generally, the physics of the relaxation of excitations in semiconductor nanocrystals receives growing interest. We show that surface defects must play an important role in these processes. We calculate the rate for the relaxation of hot carriers by impact ionization and we show that the presence of surface defects leads to an increase of the relaxation rate at lower excitation energy. We present simulations of the carrier multiplication in Si nanocrystals and we discuss the results of recent experiments in light of these results.

9:48AM P38.00006 First-principles study of LaSn3 as an anode for lithium-ion batteries. DONGWON SHIN, CHRISTOPHER WOLVERTON, Northwestern University, JOHN VAUGHHEY, MICHAEL THACKERAY, Argonne National Laboratory — Using both density functional theory (DFT) calculations and experiment, we investigate the tin-rich intermetallic compound LaSn3 as a possible anode for lithium-ion batteries. We use DFT calculations to compute the relative energies of structural insertion- and displacement-type reactions in an effort to elucidate the energetically-preferred reaction mechanism of Li with LaSn3. From our DFT calculations, we find: (i) lithium insertion reactions with LaSn3 are predicted to be energetically unfavorable and highly unlikely to occur; (ii) in contrast, the energetically preferred reaction is a displacement reaction in which Li is partially displaced from LaSn3 to yield La2Sn5 and Li reacts with the residual Sn to form Li2Sn4, corresponding to an electrochemical capacity of 307 mAh/g; (iii) this partial displacement reaction is preferred relative to the complete displacement and lithiation of Sn; and (iv) the lithiated-tin compound, Li2Sn5, is energetically much smaller favored than the commonly reported Li2Sn composition. Electrochemical and structural data largely confirm the DFT predictions; they demonstrate that lithium reacts with LaSn3 via a displacement reaction to provide a reversible specific capacity of 200-250 mAh/g.

10:00AM P38.00007 Ab Initio Prediction of the Size-Dependence of Nano-scale Platinum Dissolution in Water. KRISTIN PERSSON, LBNL, BYUNGCHAN HAN, GERBRAND CEDER, MIT — In low-temperature fuel cells, the mechanism behind the observed performance loss of the platinum catalyst is not well understood. Using ab initio methods, we calculate 0.5-2 nm diameter Pt nanoparticles with varying degrees of O and OH surface absorbates, optimized by site and particle surface structure. In fuel cells, the oxidation of the particle surface origins from the breakup of water molecules. To mimic these conditions we employ a grand canonical ensemble treatment of water as a source of O and H. Additionally, pH effects and dissolved species (from experiments) are incorporated, the latter by changing the experimental element reference state to that of calculated solids. This formalism allows us to determine the stability regions of nanoparticle Pt in equilibrium with water, as a function of particle size, potential and pH. As a result we find enhanced dissolution for the smaller Pt nanoparticles, compared to the larger. Furthermore, surface passivation effects from O and OH adsorption do not significantly increase the stability of the nano-particle phases in the potential-pH region relevant for fuel cell operating conditions. Thus, we can identify size-dependent dissolution as a mechanism which will promote the growth of larger particles at the expense of smaller ones and ultimately cause a degradation in the nanoparticle Pt catalyst performance.

10:12AM P38.00008 First-principles theory of capacitive and electrochemical energy storage. JOONGO KANG, YONG-HYUN KIM, National Renewable Energy Laboratory, Golden, CO 80401 — Recently there has been much interest in development of new electrochemical capacitors to meet high-power and high-energy applications. Pseudo-capacitors using fast surface redox reactions can store electrical energy of 10 to 100 times larger than supercapacitors and exhibit fast and reversible charge-discharge responses in contrast to batteries. Yet, energy storage mechanisms in super- and pseudo-capacitors have not been fully understood at the level of electrons. Here we have performed first-principles calculations for electrochemical double layers of a TiO2 (101) electrode and solvated lithium ions on the surface, with the ethylene carbonates (EC) as solvent molecules. As Li ions are desolvated from Li-EC2 to Li-EC3 and bare Li ions, the capacitance gets larger due to the reduced distance between the Li ions and the electrode. When Li ions are intercalated into the surface of the TiO2 electrode as supported in pseudocapacitors, the electrostatic energy due to charge separation is reduced for a given stored charge, but the electrochemical reaction starts to occur causing a large increase in the capacitance.

10:24AM P38.00009 Steps in hydrogen production from methanol on sub-nanometer palladium clusters. FAISAL MEHMOOD1, JEFFREY P. GREELEY, PETER ZAPOL1, LARRY A. CURTIS1,2, 1 Material Science Division and 2Center of Nanoscale Materials, Argonne National Laboratory — Extensive experimental and theoretical work has been done to understand the decomposition of methanol on various metal and metal oxide nanoparticles for hydrogen production. The activity of sub-nanometer sized particles <1nm however is not very well known, primarily because of technical challenges involved in preparation and stabilization of the clusters. To explore the properties of the Pd clusters computationally, we have carried out density functional calculations for the methanol decomposition reaction on Pd4 and Pd8 clusters. The thermodynamics and kinetics of three decomposition routes involving C–O, C–H and O–H scission were determined with the nudged elastic band method. A detailed analysis of the PES for methanol decomposition shows C–O activation to be the least favorable step. In addition, all possible reaction paths for the Pd4 cluster are much lower in comparison to single crystal surface and large nanoparticles. A detailed analysis of how particle size affects the elementary reaction steps, we also present a comparison of methanol decomposition on Pd4 with Pd8 clusters. Finally, we will discuss the implication of a linear correlation between the transition state and final state energies that is followed for all elementary reaction steps on Pd4 and Pd8 clusters.


10:48AM P38.00011 Electrochemical Double Layer Capacitors Using Aligned Multiwall Carbon Nanotubes Grown Directly on Conductive Substrates. RAKESH SHAH, XIANFENG ZHANG, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale, IL, 62901 — We report on the properties of Electrochemical Double Layer Capacitor (EDLCs) electrodes fabricated using aligned multiwall carbon nanotubes (MWN) grown on Ioncon sheets. Air assisted chemical vapor deposition technique was employed to synthesize the aligned MWN on these substrates. The capacitive behavior of the EDLC’s fabricated using different lengths of aligned MWNs was examined using cyclic voltammetry, constant current charge/discharge, and impedance spectroscopy. These measurements show that the charge storage phenomenon was non-Ohmic with equivalent series resistance in the range of 0.130-0.40. The maximum values of specific capacitance of the carbon nanotubes material used in these devices were in the range of 14.6-21.57 F/g. The maximum value of power density and energy density of the whole supercapacitor devices were 1.48 Wh/Kg and 2.7 kW/Kg, respectively. These results show that the multiwall carbon nanotubes grown directly on conductive substrates are promising results as electrodes for electrochemical energy storage device applications.
8:00AM P39.00001 Statistical analysis and modeling of collective cell motion and pattern formation1, ANDRAS CZIROK, ANDRAS SZABO, Eotvos University, Dept of Biological Physics — Cell motility and its guidance through cell-cell contacts is instrumental in vasculogenesis and in several other morphogenic processes as well. During vasculogenesis multicellular sprouts invade avascular areas, eventually creating an interconnected network pattern. Epithelial cell sheets migrate during organogenesis or wound healing. These phenomena were studied with time-lapse microscopy both in vivo and in vitro. Statistical analysis of cell trajectories reveals that motile confluent cultures may behave either as vortical fluids or as deforming elastic sheets. The observed flow fields and pattern formation can be explained by our generalized cellular Potts model — representing cell polarization and self-propulsion, links between the cytoskeleton of adjacent cells as well as an asymmetric preferential attraction to the surface of adjacent cells.

1This work was funded by the NIH and the Hungarian National Office for Research and Technology.

8:12AM P39.00002 Self-organization in Systems of Treadmilling Filaments., KONSTANTIN DOUBROVIN-SKI, Princeton University, KARSTEN KRUSE, Universität des Saarlandes — The cytoskeleton is an active intracellular network of polar filaments responsible for maintenance of cell shape, cell division, and cell locomotion. A broad variety of cellular processes depend critically on the ability of cytoskeletal filaments to treadmIll, i.e., to move by growing at one end while simultaneously shrinking at the other end. In particular, treadmilling is indispensable for cell crawling as well as for generation of various cellular appendages including stereocilia, microvilli, and filopodia. Quantitative modeling of systems involving treadmilling filaments is challenging since it requires describing long-range interactions of particles with many degrees of freedom. We introduce a novel framework for describing systems of treadmilling filaments. Within our framework, we identify a class of systems that admit exact solution of the underlying dynamic equations. We compare the corresponding solutions to those obtained by coarse-graining, an approximation which is valid on large length-scales. We apply our new framework to treat two biological systems: cytoskeletal dynamics in fish melanophores and locomotion of human neutrophil cells. In both cases our theory faithfully accounts for the qualitative and semi-quantitative properties of the intracellular structures observed in the corresponding experiments.

8:24AM P39.00003 Self-assembly of the yeast actomyosin contractile ring as an aggregation process: kinetics of formation and instability regimes1, NIKOLA OJKIC, DIMITRIOS VAVYLONIS, Department of Physics, Lehigh University — Fission yeast cells assemble an equatorial contractile ring for cytokinesis, the last step of mitosis. The ring assembles from ~ 65 membrane-bound “nodes” containing myosin motors and other proteins. Actin filaments that grow out from the nodes establish transient connections among the nodes and aid in pulling them together in a process that appears as pair-wise attraction (Vavylonis et al. Science 97:319, 2008). We used scaling arguments, coarse grained stability analysis of homogeneous states, and Monte Carlo simulations of simple models, to explore the conditions that yield fast and efficient ring formation, as opposed to formation of isolated clumps. We described our results as a function of: number of nodes, rate of establishing connections, range of node interaction, distance traveled per node interaction and broad band width, w. Uniform cortical 2d distributions of nodes are stable over short times due to randomness of connections among nodes, but become unstable over long times due to fluctuations in the initial node distribution. Successful condensation of nodes into a ring requires sufficiently small w such that lateral contraction occurs faster than clump formation.

1NIH R21GM083928

8:36AM P39.00004 Discrete and continuous models of protein sorting in the Golgi, HAUJUN GONG, Department of Physics, Carnegie Mellon University, RUSSELL SCHWARTZ, Department of Biological Sciences, Carnegie Mellon University — The Golgi apparatus plays an important role in processing and sorting proteins and lipids. Golgi compartments constantly exchange material with each other and with other cellular components, allowing them to maintain and reform distinct identities despite dramatic changes in structure and size during cell division, development, and secretory stress. We have developed two minimal models of membrane and protein exchange in the Golgi — a discrete, stochastic model [1] and a continuous ordinary differential equation (ODE) model — both based on two fundamental mechanisms: vesicle-coat-mediated selective concentration of soluble N-ethylmaleimide-sensitive factor attachment protein receptor (SNARE) proteins during vesicle formation and SNARE-mediated selective fusion of vesicles. Both show similar ability to establish and maintain distinct identities over broad parameter ranges, but they diverge in extreme conditions where Golgi collapse and reassembly may be observed. By exploring where the models differ, we hope to better identify those features essential to minimal models of various Golgi behaviors. [1] H. Gong, D. Sengupta, A. D. Linsteadt, R. Schwartz. Biophys J. 95: 1674-1688, 2008.

8:48AM P39.00005 ABSTRACT WITHDRAWN —

9:00AM P39.00006 Studying the Transition to Multicellular Life by Altering a Chemical Signaling Channel, CARL FRANCK, KAYVON DAIE, Cornell University — The starvation response of the eukaryotic microbial system Dictyostelium discoideum has continued to provide opportunities to explore the transition from solitary to collective life. Specifically, one observes a change of behavior from random to synchronized cellular motion reflecting successful long-ranged chemical signaling that leads to aggregation. In the typical experimental universe life goes on upon a flat substrate underneath an ocean of liquid media through which these chemical signals pass. In our observations of starvation development we have uniquely exploited the possibilities afforded by varying the depth of this signaling channel over an interesting range: from essentially infinitely thick (mm’s of depth) to an extremely thin wetting layer (below 1 micron). We also examine the development system over a wide range of surface density: from almost a full monolayer to a few percent areal coverage. Our key observation is a striking reduction of the time from the beginning of starvation to the onset of synchronized movement when we reduce the aqueous overlayer thickness to the thinnest values. We provide an interpretation for our observations by combining our results with a new framework describing systems of vortical fluids or deforming elastic sheets. The observed flow fields and pattern formation can be explained by our generalized cellular Potts model — representing cell polarization and self-propulsion, links between the cytoskeleton of adjacent cells as well as an asymmetric preferential attraction to the surface of adjacent cells.

9:12AM P39.00007 Simulation of cellular shapes on micro-patterned substrate using the Cellular Potts Model, BENOIT VIANAY, HERVE GUILLOU, Institut Neel - CNRS Grenoble - FRANCE, THERMODYNAMIC OF SMALL SYSTEMS TEAM — Cell adhesion and motility are processes involved in fundamental biological phenomena using biological structures as anchorage points and cytoskeleton filaments which are very dynamical and at non-equilibrium. We study cell adhesion on micro-patterned substrate where an introduction of a finite distance between anchorage points of the cell modifies drastically the organization of the cytoskeleton and the anchorage point’s distribution. Some of statistically most used shapes represent stationary states of the system which should minimize the energy dissipation. We verified this hypothesis reproducing morphologies by simulation of Monte Carlo using the Cellular Potts Model (Graner and Glazier, PRL69 p2013 (1992)). Shapes obtained by simulation depend of four phenomenological parameters as interaction between cell and ECM and are in excellent qualitative agreement with experimental shapes. The aim of this presented work is to link model parameters to physico-chemical properties of cells and to establish phenomenological relations between interesting parameters controlling the cytoskeleton organization. Collaborations : J. Kafer & F. Graner : Laboratoire de spectrometrie Physique – Grenoble; E. Plannus & M. Block : Institut Albert Bonniot – Grenoble.
or percolate through the entire population, leading to what might be considered as “homologous” traits even in species widely separated in morphospace.

The spread of inherited traits through the overall population, finding an “all or none” effect in which the properties of a traced organism either die out completely or persist indefinitely.

We have investigated as a function of the degree of variability, or “noise”, allowed in the morphology of new (children) organisms with respect to their parents. We find that the number of organisms in close proximity. The clustering of organisms in a morphospace overlaid on this landscape is considered an analog of speciation and is explored using analytical and numerical methods.

The bacterial strain

and shape during the early stages of Bacillus Subtilis subunit growth, simultaneously monitoring matrix expression levels. We show that the critical bioluminescence size scales with nutrient concentration as expected by a simple nutrient depletion model.

The ability of cells to move towards environmental cues is a critical process allowing the destruction of intruders by the immune system, the formation of the vascular system and the whole scale remodeling of tissues during embryo development. We examine the initial transition from single cell to group migration in the social amoeba Dictyostelium discoideum. Upon starvation, D. discoideum cells enter into a developmental program that triggers solitary cells to aggregate into a multicellular structure. The aggregation is mediated by the small molecule, cyclic-AMP, that cells sense, synthesize, secrete and migrate towards.

We obtain exact expressions for all these quantities, which we test using Monte Carlo simulations.

We study the stochastic dynamics of growth and shrinkage of single actin filaments or microtubules taking into account insertion, removal, and ATP/GTP hydrolysis of subunits. The resulting phase diagram contains three different phases: two phases of unbounded growth: a rapidly growing phase and an intermediate phase, and one bounded growth phase. We analyze all these phases, with an emphasis on the bounded growth phase. We also discuss how hydrolysis affects force-velocity curves. The bounded growth phase shows features of dynamic instability, which we characterize in the time needed for the ATP/GTP cap to disappear as well as the time needed for the filament to reach a length of zero (i.e., to collapse) for the first time. We obtain exact expressions for all these quantities, which we test using Monte Carlo simulations.

We quantify their structure using Edwards’ statistical mechanics of cellular systems.

We study 2D polygonal tilings as models of the en-face structure of single-layer biological tissues. Using numerical simulations, we explore the phase diagram of equilibrium tilings of equal-area, equal-perimeter convex polygons whose energy is independent of their shape. We identify 3 distinct phases, which are all observed in simple epithelial tissues: The disordered phase of polygons with 4-9 sides, the hexatic phase, and the hexagonal phase with perfect 6-fold coordination. We quantify their structure using Edwards’ statistical mechanics of cellular systems.

The sub-cellular oscillation of Min proteins. MinD interacts with the membrane and polymerizes into filaments. MinE binds to membrane bound MinD leading to the sub-cellular oscillation of Min proteins. MinD interacts with the membrane and polymerizes into filaments. MinE binds to membrane bound MinD leading to the self-organization of the MinD filaments. It has been observed experimentally that MinE forms a ring, known as the E-ring, near the end of the MinD polymers. We model and solve the self-organization of the E-ring. Rebinding of MinE to depolymerizing MinD filament tips controls MinE ring formation. We find two types of E-ring profiles near the filament tip: a strong plate-like E-ring as seen in vivo, controlled by 1D diffusion along the bacterial length, or a weak cup-like E-ring controlled by 3D diffusion near the filament tip. We discuss the initial instability that leads to MinD filament depolymerization and the formation of the E-ring. We also discuss the duration of transients leading towards strong or weak E-rings. We compare with experiment both in vivo and in vitro.

Upon starvation, D. discoideum cells enter into a developmental program that triggers solitary cells to aggregate into a multicellular structure. The aggregation is mediated by the small molecule, cyclic-AMP, that cells sense, synthesize, secrete and migrate towards in a head-to-tail fashion, which is changed periodically either by random fluctuations, or via a feedback mechanism based on the number of organisms in close proximity. The clustering of organisms in a morphospace overlaid on this landscape is considered an analog of speciation and is investigated as a function of the degree of variability, or “noise”, allowed in the morphology of new (children) organisms with respect to their parents. We find that a maximum number of species are formed at an intermediate value of this noise parameter, suggesting a stochastic resonance-like effect. We also address the spread of inherited traits through the overall population, finding an “all or none” effect in which the properties of a traced organism either die out completely or percolate through the entire population, leading to what might be considered as “homologous” traits even in species widely separated in morphospace.
8:12AM P40.00002 Cyclic Process as a Tool for Considering Evolution, VICTOR BONDARENKO, WSU
- Evolution is the process. The primary question is which tools we use to consider the process. In this work, basing on the original results of investigation of the intrinsic bistability in quantum systems, the concept of the cyclic process is developed for qualitative and quantitative consideration of processes as following: Everything that happens is the process of changing; the process is the cyclic process of "... → seed → plant → seed →..." type; the cyclic process is formed by two complement phase transitions of "seed → plant" and "plant → seed" type; the cyclic process is the manifestation of self-consistent interaction of interdependent two-state system, environment, and radiation, so that the whole Universe is involved in each process; the cyclic process can be described qualitatively and quantitatively by a real cubic equation with four generalized dimensionless real parameters, provided that one of the parameters undertakes cyclic change of its value and all four parameters belong to limited interdependent intervals to maintain cyclic process. Using the cyclic process approach as a powerful tool a variety of issues is considered. Preference of evolution, extinction, adaptation, and relation between microscopic structure and macroscopic behavior of the system are addressed. Seeing the evolution is the most transcending seeing of existence. The cyclic process approach is suggested to be a corner stone for scientific approach to seeing evolution.

8:24AM P40.00003 Stepping in the bacterial flagellar motor, THIERRY MORA, HOWARD YU, NED S. WINGREEN, Princeton University - Many bacteria swim by virtue of tiny rotary motors that drive rotation of helical flagella. These motors are powered by a proton flux that is converted into torque by a mechanism which remains largely unknown. Recently, it has been reported that at low speed, the bacterial flagellar motor proceeds by steps. To account for these steps, we propose a physical model in which the stator drives a "bumpy" rotor through a viscous medium. Our model is consistent with most of the available data, and allows us to make testable predictions, in particular on the speed and diffusion properties of the rotor.

8:36AM P40.00004 Actin-Polymerization-Driven Motility with Site Specific Tethering, EDWARD BANIGAN, ANDREA LIU, University of Pennsylvania - A recent numerical simulation by Lee and Liu (2008) has demonstrated a new possible mechanism for actin-polymerization-driven motility. The simulation is a physically consistent version of the Brownian dynamics formulation of the dendritic nucleation model. The model shows that motility can indeed be achieved with the constituent proteins of the dendritic nucleation model, but that motility arises from a mechanism completely different from those proposed before. In the simulations, thebuild-up of F-actin behind the moving surface drives the surface forwards if the surface has a net repulsion with actin. In this work, we extend the model to include a site specific tethering interaction between the moving surface and actin, to imitate, for example, the effects the Acta or N-Wasp protein. We study the effects of varying binding strength and binding site coverage.

8:48AM P40.00005 FKBP binding free energies obtained via non-equilibrium simulation, F. MARTY YTREBERG, University of Idaho - We discuss the advantages and disadvantages of estimating binding free energies (i.e., absolute binding affinities) via non-equilibrium unfolding simulations. The study utilizes the FKBP protein bound to two different ligands as a model system. The non-equilibrium methodology utilized is straightforward, requiring little or no modification to modern molecular simulation packages, and is trivially parallelizable. The approach makes use of a physical pathway, eliminating the need for complicated alchemical decoupling schemes.

9:00AM P40.00006 Computational Research Needs for Renewable and Alternative Energy: Studies of Natural and Artificial Photosynthesis, VICTOR BATISTA, Yale University - The atmospheric oxygen that sustains life on earth has been generated by plants during the light period of photosynthesis. At the molecular level, the reaction involves catalytic water splitting into dioxygen, protons and electrons in the subunit D1 of photosystem II (a transmembrane complex of about 20 proteins found in the thylakoid membranes of green plant chloroplasts). Both the reaction mechanism and the structure of the catalytic center responsible for this important reaction remain poorly understood. This talk will present recent advances in experimental and computational studies towards the development of rigorous models of the oxomanganese catalytic complex and the catalytic cycle responsible for oxygen evolution, as well as recent progress on studies of biomimetic systems for artificial photosynthesis.

9:12AM P40.00007 Systematic Coarse-Graining of Peptides to Understand their Effective Molecular Interactions, LUCA LARINI, GREGORY A. VOTH, Center for Biophysical Modeling and Simulation and Department of Chemistry, University of Utah, Salt Lake City, UT, 84112, USA - The process of building reliable coarse-grained models is a major challenge for both theory and simulation. Force matching is a systematic method to produce quantitatively accurate coarse-grained potentials from atomistic simulation data. This method provides a sound theoretical background that can also be used to gain deeper insight into the system under examination. In this way, force matching can be employed as a tool for analysis. Application to a simple biological molecule will be described in order to gain a better understanding of the effective forces acting on the system.

9:24AM P40.00008 Rigorous treatment of electrostatics for spatially varying dielectrics: how far can one go using energy minimization?, YI-KUO YU, OLEG OBOLENSKY, RAJARSHI RAY, T. DOERR, National Center for Biotechnology Information/NIH - A novel energy minimization formulation of electrostatics that allows computation of the electrostatic energy and forces to any desired accuracy in a system with arbitrary dielectric properties is presented. An integral equation for the scalar charge density is derived from an energy functional of the polarization vector field. This energy functional represents the true energy of the system even in non-equilibrium states. Arbitrary accuracy is achieved by solving the integral equation for the charge density via a series expansion in terms of the equation's kernel, which depends only on the geometry of the dielectrics. The streamlined formalism operates with volume charge distributions only, not resorting to introducing surface charges by hand. Therefore, it can be applied to arbitrary spatial variation of the dielectric susceptibility. The simplicity of calculation of the formalism to real problems is shown with three examples.

We thank the administrative group of the NIH Biowulf clusters, where all the computational tasks were carried out. This research was supported by the Intramural Research Program of the NIH, NLM.

9:36AM P40.00009 Ab-Initio Based Computation of Rate Constants of Spin Forbidden Transitions in (Bio)inorganic Complexes and Metalloproteins, ABDULLAH OZKANLAR, JORGE H. RODRIGUEZ - Some (bio)chemical reactions are non-adiabatic processes whereby the total spin angular momentum, before and after the reaction, is not conserved. These are named spin- forbidden reactions. The application of spin density functional theory (SDFT) to the prediction of rate constants is a challenging task of fundamental and practical importance. We apply non-adiabatic transition state theory in conjunction with SDFT to predict the rate constant of the spin- forbidden didehydrogen binding to iron tetracarbonyl. To model the surface hopping probability between singlet and triplet states, the Landau-Zener formalism is used. The lowest energy point for singlet-triplet crossing, known as minimum energy crossing point (MECP), was located and used to compute, in a semi-quantum approach, reaction rate constants at 300 K. The predicted rates are in good agreement with experiment. In addition, we present results which are relevant to the ligand binding reactions of metalloproteins. This work is supported in part by NSF via CAREER award CHE-0349189 (JHR).

1 Department of Physics, Purdue University, West Lafayette, IN 47907-2036
9:48AM P40.00010 Electrostatic properties of two finite width charged dielectric slabs in water, Y.S. IHO, UCSB, M. KANDUC, SI-1000 Ljubljana, A. NAJI, UCSB, M.W. KIM, KAIST/UCSB, R. PODGORNIK, SI-1000 Ljubljana, F.L.H. BROWN, P.A. PINCUS, UCSB — We study the electrostatic interaction between two like-charged membranes of finite thickness embedded (composed of five parallel dielectric interfaces) in a medium of higher dielectric constant. A generalized SC theory is applied along with extensive Monte-Carlo simulations which applied numerical algorithm based on the image charge method to calculate accurate electrostatic potential or forces. We found the dielectric discontinuity is important in a SC regime. They drive strong counterion crowding in the central region of the inter-surface space upon increasing the solvent/membrane dielectric mismatch and change the membrane interactions from attractive to repulsive at small separations.

10:00AM P40.00011 Electronic Structure Analysis for Proteins on the FMO Method, TOMOKI KOBORI, SHINJI TSUNEYUKI, KEITARO SODEYAMA, University of Tokyo, KAZUTO AKAGI, Tohoku University, KIYOHUKE TERAKURA, JAIST, HIDETOSHI FUKUYAMA, Tokyo University of Science — The enormity and complexity of proteins have rendered their electronic structure calculation very costly. Although recently established Fragment Molecular Orbital (FMO) method enables us to calculate total energy of a huge protein precisely based on quantum mechanics, the method does not refer to one-electron orbitals and one-electron energy spectrum. In this paper we propose a method of analyzing electronic structure of a protein based on first principles calculation with reasonable accuracy and CPU cost. We construct one-electron Hamiltonian of proteins by assembling the output of the FMO method: fragment orbitals are determined by fragment monomer calculation, while interaction and overlap between fragment orbitals in different fragments are obtained from dimer calculation. After one-electron Hamiltonian matrix of the whole system is fabricated with the fragment orbital basis, one-electron energy spectrum is obtained by its diagonalization. If the matrix dimension is too large, unimportant orbitals are eliminated from the matrix so that the diagonalization of the Hamiltonian becomes feasible. The method is applicable to both the Hartree-Fock method and the density functional theory. In this paper, validity of the method is verified by some test calculations of small peptides.

10:12AM P40.00012 Helical secondary structure of polyalanine peptides in vacuo: Ac-Ala$\alpha$-LysH$^+$ ($n=5,10,15$), experiment and theory, MARIANA ROSSI, VOLKER BLUM, PETER KUPSER, GERT VON HELDEN, FRAUKE BIERAU, GERARD MEULER, MATTHIAS SCHEFFLER, Fritz Haber Institute, D-14195 Berlin, Germany — The presence of a solvent is often viewed as indispensable to quantify the stabilization interactions. However, well defined secondary structure motifs (helices, sheets, ...) also exist in vacuo, offering a unique “clean room” condition to quantify the stabilizing interactions. We here unravel the structure of Lysine$^+$ capped polyalanine peptides Ac-Ala$\alpha$-LysH$^+$ ($n=5,10,15$), by combining experimental multi-photon IR spectra obtained using the FELIX free-electron laser at room-temperature with van der Waals-corrected all-electron density-functional theory (DFT) in the generalized gradient approximation in the FHI-aims code [1]. Earlier ion mobility studies of these molecules indicate helical structure [2], which we here demonstrate quantitatively. For $n=5$, we find a close energetic competition of different helix motifs ($\alpha$, $3_1\beta$), with similar and good agreement between measured and calculated vibrational spectra. We show how the Lys$^+$ termination acts to induce helices also for longer peptides, and how vibrational modes develop with helix length ($n=10,15$), yielding, e.g., a softening of collective modes towards the infinite helix limit. [1] V. Blum et al, Comp. Phys. Comm. (2008), accepted. [2] M. Kohtani et al., JACS 120, 12975 (1998).

10:24AM P40.00013 Hofmeister effect and the phase diagram of lysozyme, STEVEN LETTIERI, XIAOFEI LI, JAMES GUNTON, Lehigh University — The phase diagrams for lysozyme are calculated for two different precipitant salts, NaCl and NaSCN, using a potential of mean force that takes into account contributions from ion-dispersion forces (J.Phys.Chem.B, 110, 24757). Our results are consistent with a recent perturbation theory calculation (J.Phys.Chem.B, 110, 24775) in that the phase diagram for lysozyme with NaCl is quite different than for lysozyme with NaSCN for the same molar concentration (0.2M). However, in contrast to the perturbation theory calculation, we find that the lysozyme phase diagram with NaCl has a metastable fluid-fluid coexistence curve and that the metastability gap in the case of NaSCN is much larger than predicted by perturbation theory.

1This work was supported by grants from Harold G. and Leila Y. Mathers Charitable Foundation and the National Science Foundation.

10:36AM P40.00014 Infrared Spectroscopy with ab initio molecular dynamics simulations : gas phase floppy peptides of increasing size and complexity, in relation with IR-MPD experiments, MARIE-PIERRE GAEGOT, Universite d’Evry val d’Essonne - LAMBE UMR8887, IR-MPD EXPS, GILLES GREGOIRE & J.P. SCHERMANN COLLABORATION, IR-MPD EXPS, L. SNOEK & T. VADEN COLLABORATION — We present finite temperature DFT-based Car-Parrinello molecular dynamics (MD) simulations for the calculation of infrared spectra of complex molecular systems, either in the gas phase or in the condensed phase. We will review the fundamentals of the method, as well as the applicability and originality of finite temperature MD simulations for the purpose of modeling infrared spectra. Illustrations are taken from the fundamentals of infrared spectroscopy of alanine peptides of increasing size and complexity (from dipeptides to an octo-peptide) in the gas phase, in relation with IR-MPD (Infrared Multi Photon Dissociation) experiments : 300-400 K gas-phase action spectroscopy as devised on the CLIO platform at the University of Orsay-France or on the platform developed in the group of L. Snoek at Oxford-UK. A special emphasis on vibrational anharmonicities and how they can be extracted from molecular dynamics simulations will be put forward. Furthermore, band assignments in terms of atomic movements from MD is challenging and we have introduced a general method for obtaining effective normal modes of molecular systems from MD simulations.

10:48AM P40.00015 Linear irreversible thermodynamics, efficiency and coefficient of performance of a thermal Brownian motor in tight coupling, MULUGETA BEKELE, ANTENEH GETACHEW, Department of Physics, Addis Ababa University, Addis Ababa, Ethiopia, ARUN JAYANNVAR, Institute of Physics, Sachivalaya Marg, Bhubaneswar, India — We analytically calculated the Onsager’s coefficients near a finite stall force in the spirit of recent development in non-equilibrium steady state thermodynamics. We show that the occupancy relation holds and the determinant of the Onsager’s matrix vanishes when heat leakage is neglected. This condition implies that the device is built with tight coupling and hence Carnot’s efficiency can be achieved for the quasi-static process. We also show that the efficiency at maximum power to be exactly half of Carnot’s efficiency. Under similar condition we explore the coefficient of performance when our model works as a refrigerator.

1International Programme in Physical Sciences, Uppsala University, Uppsala, Sweden and Office of External Affairs, ICTP, Trieste, Italy. Wednesday, March 18, 2009 8:00AM - 10:48AM Session P41 DCMP DMP: Models of Strongly Correlated Electrons 413
8:00AM P41.00001 Time-Reversal Symmetry Breaking and Spontaneous Anomalous Hall Effect in Fermi Fluids, KAI SUN, EDUARDO FRADKIN, UIUC — We study the spontaneous non-magnetic time-reversal symmetry breaking in a 2D Fermi liquid without breaking either the translational symmetry or the $U(1)$ charge symmetry. Using a Berry phase approach, we found that for a large class of models, including all one- and two-band models, the time-reversal symmetry breaking states can be classified into two classes, dubbed type I and II, depending on the accompanying spatial symmetry breaking patterns. The properties of each class are studied. In particular, we show that the states breaking both time-reversal and chiral symmetries (type II) are described by spontaneously generated Berry phases and exhibit anomalous Hall effect in the absence of magnetic fields and magnetic impurities. We also show examples of the time-reversal symmetry breaking phases in several different microscopically motivated models and calculate their associated Hall conductance within a mean-field approximation. In particularly, we found a simple lattice structure in which the time-reversal symmetry breaking phases is stabilized by infinitesimal interactions.

8:12AM P41.00002 String-nets, quantum loop gases and the sign problem for non-abelian anyons, ANDREA VELENICH, CLAUDIO CHAMON, Boston University, XIAO-GANG WEN, M.I.T. — Hamiltonians giving rise to topological ground states can be constructed explicitly as sums of local operators acting on Hilbert spaces where distinct classical string-net configurations are orthogonal. We show explicitly the connection between string-nets and quantum loop gas models with their non-orthogonal inner product. Also we emphasize the role of the “sign problem” for a Hamiltonian in enforcing the topological character of its ground state.

8:24AM P41.00003 Hydrodynamic description of spin Calogero-Sutherland model, ALEXANDER ABANOV, Stony Brook University, MANAS KULKARNI, Stony Brook University and Brookhaven National Laboratory, FABIO FRANCHINI, The Abdus Salam ICTP — We study a non-linear collective field theory for an integrable spin-Calogero-Sutherland model. The hydrodynamic description of this $SU(2)$ model in terms of charge density, charge velocity and spin currents is used to study non-perturbative solutions (solitons) and examine their correspondence with quantum numbers of elementary excitations [1]. A conventional linear bosonization or harmonic approximation is not sufficient to describe, for example, the physics of spin-charge (non-)separation. Therefore, we need this new collective bosonic field description that captures the effects of the band curvature. In the strong coupling limit [2] this model reduces to integrable $SU(2)$ Haldane-Shastry model. We study a non-linear coupling of left and right spin currents which form a Kac-Moody algebra. Our quantum hydrodynamic description for the spin case is an extension for the one found in the spinless version in [3].


8:36AM P41.00004 Supersymmetry in strongly correlated fermion models, DIMITRIS GALANAKIS, University of Illinois at Urbana - Champaign, STEFANOS PAPANICOLAOU, CHRIS HENLEY, Cornell University — We investigate the Fendley and Schoutens model of hard core fermions on lattice which have hopping elements $t$, and potential terms $V$ which include a second-neighbor repulsion with some multi-particle terms. At the special point $t = V$, they showed that the Hamiltonian is $H = (Q_t^\dagger (r), Q_t)$ with $Q = \sum q(r) = \sum c(r)^* P(r)$, where $c(r)$ is an annihilation operator and $P(r)$ enforces the hardcore. That means the system acquires an exact non-relativistic supersymmetry, and for a range of fillings has a large number of zero-energy ground state [1]. To obtain insights on the nature of the zero-energy states and excitations, we perform exact diagonalization studies on finite clusters for various interaction strengths, fillings and lattice geometries. We note that for fillings beyond $n \approx 0.3$, we find coexisting domains of the inert crystal at $n = 1/2$, in contrast to a related non-supersymmetric model [2]. Moreover, using both numerical and analytical tools, we investigate perturbative limits where $q(r)$ is changed so as to preserve supersymmetry but a particular class of ground-states becomes trivial.


8:48AM P41.00005 Hexatic and Microemulsion Phases in the 2d Quantum Plasma, BRYAN CLARK, Department of Physics, University of Illinois at Urbana Champaign, MICHELE CASULA, Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau, France, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana Champaign — It has been long known that the two-dimensional one component plasma supports both a Wigner-crystal and liquid phase. Classically [1,2], it is known that a hexatic phase exists but it is not known how this hexatic phase extends into the quantum regime. Moreover, at low temperature, phenomenological arguments [3] from Jamiei, et. al. suggest the existence of microscopic phases including stripes and bubbles. We use diffusion and path integral Monte Carlo to map out this phase diagram. We are able to extend the hexatic phase into the quantum regime as well as quantify the nature of the defects and exponents in the long range quantum system. We also specify the nature, extent and existence (or lack thereof) of the expected low-T microemulsion phases. We use diffusion and path integral Monte Carlo to map out this phase diagram. We are able to extend the hexatic phase into the quantum regime as well as quantify the nature of the defects and exponents in the long range quantum system. We also specify the nature, extent and existence (or lack thereof) of the expected low-T microemulsion phases.


9:00AM P41.00006 Quantum phase transition in a staggered flux phase, CHRISTOPH PUETTER, HAE-YOUNG KEE, University of Toronto — We study the quantum critical point inside the staggered flux phase. We present the dynamics of the fermions at the critical point and discuss their relevance for the phenomena observed in high-Tc cuprates.

9:12AM P41.00007 Quantum correlated percolation, LIANG CAO, Syracuse University, M. JENG, Microsoft Corporation, J. M. SCHWARZ, Syracuse University — Abstract: Quantum percolation is the study of hopping transport of a quantum particle on randomly diluted percolation clusters. Inspired by correlated percolation models of geometrical jamming, we extend quantum percolation to investigate hopping transport on percolation clusters with geometric constraints on the occupation of bonds/sites. An example of a geometric constraint is each occupied site must have at least two occupied neighboring sites to remain occupied ($k$-core percolation). Another example is particular sets of neighboring sites containing at least one occupied site for an occupied site to remain occupied (spiral model). Both models exhibit long-range geometrical correlations differing from ordinary percolation and give rise to a discontinuous phase transition (in high dimensions for $k$-core percolation). To investigate how these atypical long-range geometrical correlations affect the hopping transport of a quantum particle, we numerically study the level statistics of quantum $k$-core percolation on the Bethe lattice and the two-dimensional quantum spiral model. While the quantum $k$-core model exhibits an insulator-to-metal transition as the occupation probability is increased, preliminary results indicate that there is no insulator-to-metal transition in the two-dimensional quantum spiral model. Studies of a three-dimensional quantum spiral model will also be addressed as well possible physical applications of quantum jamming.
9:24AM P41.00008 Frustration of dissipation in a spin-boson model. KEVIN INGERSENT, ALPER DURU, U. of Florida — The spin-boson model (SBM), in which a quantum two-level system couples via one component of its effective spin to a dissipative bosonic bath, has many realizations. There has been much recent interest in the SBM with a sub-Ohmic bath characterized by a power-law spectral exponent (0 < s < 1), where at zero temperature a quantum critical point separates delocalized and localized phases. Numerical renormalization group calculations have called into question [1] the validity of the long-anticipated mapping between the SBM and the classical Ising chain with interactions decaying with distance as $|i-j|^{-s}$ as $1/|i-j|^{1+s}$. Attention has also fallen on a variant of the SBM in which two components of the impurity spin couple to different bosonic baths. For Ohmic case ($s = 1$), competition between the baths has been shown to frustrate the dissipation and reduce the coupling of the impurity to the environment [2]. The present study addresses the SBM with two sub-Ohmic baths, where dissipative effects are intrinsically stronger than for $s = 1$. Numerical renormalization group methods are used to identify a continuous quantum phase transition in this model and to evaluate critical exponents characterizing the quantum-critical behavior in the vicinity of the transition. [1] M. Vojta et al., Phys. Rev. Lett. 94, 070604 (2005). [2] E. Novais et al., Phys. Rev. B 72, 014417 (2005). Supported by NSF Grant DMR-0710540.

9:36AM P41.00009 Fidelity susceptibility and quantum phase transitions1, SHI-JIAN GU, Department of Physics, The Chinese University of Hong Kong — In this talk, I will introduce the quantum fidelity approach to quantum phase transitions based on its leading term, i.e. the fidelity susceptibility. The fidelity susceptibility denotes the adiabatic leading response of the ground state to the driving parameter. Differ from traditionally approach based on the ground-state energy, the fidelity susceptibility shows distinct scaling and singular behaviours around the critical point. I will present also the ground-state fidelity approach to both Landau’s phase transition and topological phase transition, as illustrated by the Lipkin-Meshkov-Glick model and the Kitaev honeycomb model, respectively.

1This work is supported by an Earmarked Grant for Research from the Research Grants Council of HKSAR, China (Projects No. CUHK 400906)

9:48AM P41.00010 Scaling of logarithmic quantum fidelity in the Lipkin-Meshkov-Glick model1, CHING YEE LEUNG, HONG KWOK, SHI-JIAN GU, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong — The quantum fidelity is used to describe quantum phase transitions in many works. As the classical expression of logarithmic fidelity is shown to be an extensive value, it was suggested that the logarithmic fidelity can be averaged over the system size and named as fidelity per site. However, illustrated by the anisotropic Lipkin-Meshkov-Glick model, which exhibits different scaling behaviour in different phases, we show that the logarithmic fidelity in the ground state of the model scales like $N$ in the symmetry-broken phase and $N^{0}$ in the polarizing phase. It is suggested to be a pure quantum effect and generalization of fidelity per site is proposed.

1This work is supported by an Earmarked Grant for Research from the Research Grants Council (RGC) of the HKSAR, China (Project No. CUHK204/05).

10:00AM P41.00011 Multicanonical Monte Carlo simulations of anisotropic SU(3) and SU(4) Heisenberg models, KENJI HARADA, Kyoto University, NAOKI KAWASHIMA, ISSP, University of Tokyo, MATTHIAS TROYER, ETH, Zurich — We present the results of multicanonical Monte Carlo simulations on two-dimensional anisotropic SU(3) and SU(4) Heisenberg models. In our previous study [K. Harada, et al., J. Phys. Soc. Jpn. 76, 013703 (2007)], we found evidence for a direct quantum phase transition from the valence-bond-solid (VBS) phase to the SU(3) symmetry breaking phase on the SU(3) model and we proposed the possibility of deconfined critical phenomena (DCP) [T. Senthil, et al., Science 303, 1490 (2004); T. Grover and T. Senthil, Phys. Rev. Lett. 98, 247202 (2007)]. Here we will present new results with an improved algorithm, using a multicanonical Monte Carlo algorithm. Using a flow method-like technique [A.B. Kuklov, et al., Annals of Physics 321, 1602 (2006)], we discuss the possibility of DCP in both models.

10:12AM P41.00012 Topological stability of q-deformed quantum spin chains, CHARLOTTE GILS, ETH Zurich, EDDY ARDONNE, Nordita, SIMON TREBST, Microsoft Research, Station Q, ANDREAS LUDWIG, UC Santa Barbara, MATTHIAS TROYER, ETH Zurich, ZHENGHAN WANG, Microsoft Research, Station Q — Quantum mechanical systems, whose degrees of freedom are so-called $su(2)_q$ anyons, form a bridge between ordinary spin systems and systems of interacting non-Abelian anyons. Such a connection can be made for arbitrary spin-$S$ systems, and we explicitly discuss spin-$1/2$ and spin-1 systems. Anyonic spin-$1/2$ chains exhibit a topological protection mechanism that stabilizes their gapless ground states and which vanishes only in the limit $(k \rightarrow \infty)$ where the system turns into the ordinary spin-$1/2$ Heisenberg chain. For anyonic spin-1 chains we show that their phase diagrams closely mirror the one of the biquadratic spin-1 chain. This includes generalizations of the Haldane phase, of the AKLT point, and the appearance of several stable critical phases described by (super)conformal field theories.

10:24AM P41.00013 Momentum distribution of the one-dimensional hard-core boson Hubbard model, MIN-CHUL CHA, JONG-GEUN SHIN, Hanyang University-Ansan (Korea), JI-WOO LEE, Myongji University (Korea) — We investigate the momentum distributions, $n_k$, of the one- dimensional hard-core boson Hubbard model as a function of the nearest-neighbor interaction strength by exact diagonalizations for lattices up to 30 sites. It is well known that the ground state of this model shows a quantum phase transition between the Ising-ordered insulating phase and the XY-ordered superfluid phase at $V = 2t$. Predetermination of the critical point helps us to investigate various critical behaviors. At the critical point, the momentum distribution shows a linear dependence ($n_k \sim |k - \pi|$). $n_k (k = \pi)$ shows different critical behaviors upon approaching the critical point in the Ising or XY regions. Some other properties of the momentum distributions and the critical behaviors are discussed.

10:36AM P41.00014 Ring-exchange interaction in doubly degenerate orbital system with strong electron correlation, JOJI NASU, Department of Physics, Tohoku University, SUMIO ISHIHARA COLLABORATION — Degree of freedom is one of the attractive themes in transition-metal oxides. Since the inter-site orbital interaction depends explicitly on the bond direction, one orbital configuration which minimizes the bond energy in one direction does not minimize in other directions. This is a kind of frustration. We study the $e_g$ orbital model (EOM) where the $e_g$ orbital is represented by the pseudo-spin (PS) with nearest neighbor (NN) interaction in a cubic lattice. Due to this frustration, this model shows a macroscopic number of degenerate states in the classical ground states. It is known that these states are lifted by thermal and quantum fluctuations. We examine the long-range interaction effect in the EOM. This interaction is derived by the higher-order perturbational processes of the electron transfer under strong on-site Coulomb repulsion in the two orbital Hubbard model. In particular, roles of the orbital ring-exchange interaction are focused on. This includes the magnetic octupole operator which does not appear in the previous EOM with NN interaction. We analyzed this model by the mean field approximation and the classical Monte-Carlo method. We found that PS canted state is stabilized rather than PS collinear state which is realized in the previous EOM due to thermal and quantum fluctuations. It is also shown that the magnetic octupole polarization appears in a wide parameter region.

Wednesday, March 18, 2009 11:15AM - 1:39PM — Session Q1 DCMP: Memory and Focusing in Catastrophic Deformations Spirit of Pittsburgh Ballroom A
11:15AM Q1.00001 Tsunami Asymptotics. MICHAEL BERRY, Physics Department, Bristol University, UK — Optical analogies, and some singularity theory, give new information about tsunamis. For most of their propagation, tsunamis are linear dispersive waves whose speed is limited by the depth of the ocean and which can be regarded as diffraction-decorated caustics in spacetime. For constant depth, uniform asymptotics gives a very accurate compact description of the tsunami profile generated by an arbitrary initial disturbance. Variations in depth act as lenses and can focus tsunamis onto cusped caustics, and this “singularity on a singularity” constitutes an unusual diffraction problem, whose solution indicates that focusing can amplify the tsunami energy by an order of magnitude.

11:51AM Q1.00002 Memory encoding vibrations in a disconnecting air bubble. WENDY ZHANG, University of Chicago — The implosion that disconnects a submerged air bubble into several bubbles provides a simple example of energy focusing. The most efficient disconnection is an entirely symmetric one terminating in a finite-time singularity. At the final moment, the potential energy at the start of the disconnection is entirely condensed into the kinetic energy of a vanishingly small amount of liquid rushing inwards to disconnect the bubble. In reality, however, the initial shape always possesses slight imperfections. We show that a memory of the imperfection remains and controls the final fate of the focusing. Linear stability reveals that even an infinitesimal perturbation is remembered. A slight initial asymmetry excites vibrations in the cross-section shape of the bubble neck. The vibrations persist over time. Near the singularity, their amplitudes freeze, locking onto constant values, while their frequencies chirp, increasing more and more rapidly. The net effect is that the singularity remembers exactly half of the information about the initial imperfection, the half encoded by the vibration amplitudes. We check this scenario in an experiment by releasing an air bubble from a nozzle with an oblong cross-section. This excites an elongation-compression vibrational mode. We measure the vibration excited and find quantitative agreement with linear stability. When the initial distortion has a small, but finite, size, the saturation of the vibration amplitude causes the symmetric singularity to be pre-empted by an asymmetric contact between two distant points on the interface. Numerics reveal that the contact is typically smooth, corresponding to two inward-curving portions of the bubble surface colliding at finite speed. Both the contact speed and curvature vary non-monotonically with the initial distortion size, with abrupt jumps at specific values. This is because the vibration causes contact to occur at different values of the phase. A contact produced when the shape distortion is pronounced requires a smaller initial amplitude than a contact produced when the vibration is out of phase. (Joint work with Nathan C. Keim, Lipeng Lai, Laura E. Schmidt, Konstantin Turitsyn and Sidney R. Nagel.)

12:27PM Q1.00003 Pattern Transformation Triggered by Deformation. TOM MULLIN, Manchester Centre for Nonlinear Dynamics, University of Manchester, Oxford Road, Manchester M13 9PL, UK — Periodic elastomeric cellular solids are subjected to uniaxial compression and a novel uniform transformation of the structure is found above a critical value of applied load. The results of a numerical investigation reveal that the pattern switch is triggered by a reversible elastic instability. The mechanism has proved to be useful for controlled imprinting of complex patterns in phononic and photonic crystals. The material also provides an example of a simple, tunable and robust negative Poisson ratio foam. More recently, the inverse problem of an appropriate array of elastic particles has been shown to provide another example of an intriguing pattern switch.

1:03PM Q1.00004 Resonant generation of internal waves on a model continental slope. HEPENG ZHANG, Univ. of Texas at Austin — Away from shallow, well-mixed surface regions, the density of sea water increases with depth due to variation in salinity and temperature. This continuous density stratification supports internal gravity waves, which are the counterpart within the fluid interior of surface gravity waves. Internal gravity waves are important for many oceanic processes, such as sediment transportation and ocean mixing. We study internal wave generation in a laboratory model of oscillating tidal flow on a continental margin. Waves are found to be generated only in a near-critical region where the slope of the bottom topography matches that of internal waves. Fluid motion with a velocity an order of magnitude larger than that of the forcer occurs within a thin boundary layer above the bottom surface. The resonant wave is unstable because of strong shear; Kelvin-Helmholtz billows precede wave breaking. We construct a model to extrapolate our results to oceanic conditions. This work [1] provides a new explanation for the intense boundary flows on continental slopes.

Wednesday, March 18, 2009 11:15AM - 1:39PM – Session Q2 DCMP: New Insights into Hidden Order in URu2Si2

11:15AM Q2.00001 Sleuthing Hidden Order in URu2Si2. PREMALA CHANDRA, Center for Materials Theory, Dept. of Physics and Astronomy, Rutgers University — In this talk, I will provide an overview of recent experimentally-driven advances in our understanding of the hidden order in URu2Si2; constraints and implications for future theoretical work will be discussed. State-of-the-art pressure, neutron and transport measurements [1] on this material have led to the confirmation of the phase diagram proposed on theoretical grounds for URu2Si2 several years ago [2], while recent neutron [3], ARPES and STM studies provide growing evidence for the formation of a density wave of unknown character [2]. I will also describe the challenge of linking the observed excitations to the underlying hidden order, and will discuss ongoing theoretical advances in this direction.

References:

11:51AM Q2.00002 ARPES Clues to the Hidden Order in URu2Si21. JONATHAN DENLINGER2. Lawrence Berkeley National Laboratory — The three-dimensional electronic structure of UHV-cleaved URu2Si2 is investigated using photon-dependent angle-resolved photoemission (ARPES). Wide angle Fermi-surface (FS) maps as well as high-resolution spectroscopy focused on key high symmetry points reveal high-U 5f spectral weight at the hole-like regions of the FS. ARPES is made to LDA+DMFT calculations as several years ago [2], while recent neutron [3], ARPES and STM studies provide growing evidence for the formation of a density wave of unknown character [2]. I will also describe the challenge of linking the observed excitations to the underlying hidden order, and will discuss ongoing theoretical advances in this direction.

References:
[1] Supported by the U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231), at UM (DE-FG02-07ER46379) and UCSD (FG02-04ER46105 & FG02-04ER46178), and by the NSF at UCSD (DMR08-02478).
12:27PM Q2.00003 Neutron Scattering Studies of Hidden Order in URu$_2$Si$_2$. **CHRISTOPHER WIEBE.** Florida State University/NHMFL — The heavy fermion superconductor URu$_2$Si$_2$ has held the attention of physicists for the last two decades due to the presence of a mysterious hidden order phase below 17.5 K. Previous neutron scattering measurements indicate that the ordered moment is 0.03 $\mu_B$, much too small to account for the large heat capacity anomaly at 17.5 K. We present recent neutron scattering experiments which unveil a new piece of this puzzle – the spin excitation spectrum above 17.5 K exhibits well-correlated, itinerant-like spin excitations up to at least 10 meV emanating from incommensurate wavevectors.

The gapping of these excitations corresponds to a large entropy release and explains the reduction in the electronic specific heat through the transition. We also present new neutron scattering data linking the spin excitations to Fermi surface instabilities, and discuss the remaining candidates for the identity of the hidden order phase.

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1:03PM Q2.00004 Competition of Hidden Order and Antiferromagnetism in URu$_2$Si$_2$ under Pressure. **ELENA HASSINGER, INAC, CEA Grenoble, France — URu$_2$Si$_2$ is a heavy fermion compound with an ordered phase below $T_d = 17.5$ K at ambient pressure. The signature of the transition at $T_d$ in macroscopic quantities is very large and indicates a partial gap opening on the Fermi surface. However, the order parameter could not be identified yet and therefore, the phase is called hidden order (HO). Additionally, the compound becomes superconducting below $T_{SC} = 1.4$ K. Here, we focus on the difference between HO and the pressure induced antiferromagnetic state (AF) in order to shed light on the HO itself. By specific heat and resistivity measurements under pressure we were able to confirm the pressure-temperature phase diagram determined by neutron scattering.**

For pressures higher than $P_c = 0.5$ GPa the antiferromagnetic phase develops and superconductivity is suppressed at the same time. The transition line between HO and AF can be seen as a small anomaly in resistivity and specific heat data until 1.3 GPa, where it seems to join the transition line between the paramagnetic and the HO phase. The nesting-like signature at $T_d$ in resistivity surprisingly does not change qualitatively between low pressures at the transition to HO and high pressures at the transition to the AF. The differences in the low energy excitations between the HO and AF phases have been investigated by neutron scattering measurements at 0.67 GPa where three phases can be detected on cooling: paramagnetic, HO and AF phase. The inelastic response at the antiferromagnetic wavevector $Q_H = (1,0,0)$ and at the position of the second minimum in the dispersion relation $Q_d = (1.4,0,0)$ was measured in the three distinct phases. The sharp excitation at $Q_d$ with a gap of 1.8 meV exists only in the hidden order phase and disappears in the antiferromagnetic phase whereas the excitation at $Q_1$ persists in both phases. Therefore only the excitations at the commensurate wavevector $Q_0$ are characteristic of the HO phase.

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11:15AM Q3.00001 Computerized Comparison and Analysis of Vincent van Gogh’s Painting Brushstrokes. **JAMES Z. WANG, The Pennsylvania State University — With advanced digitization techniques, museums have routinely begun to assemble vast digital libraries of images of their collections. These images can be analyzed by computers to assist art historians for a number of tasks. In our work, we focus on three challenges: artist identification, dating of an art work, and finding distinguishing features among artists. Two complementary approaches were taken: (1) the analysis of the geometric statistics based on the extracted individual brushstroke, and (2) the modeling of overall brushstroke texture.**

These approaches aim at assisting art historians in comparing a painting or parts of a painting to a group of paintings based on multiple criteria. Statistical methods have been used to compare groups of paintings. Each painting image is divided into subimages. Individual brushstrokes are segmented automatically. Geometric features, including the curvature, the overall orientation, and the size, are computed for each brushstroke. We also compute the features representing the interaction of the brushstrokes extracted. The statistics, including average and standard deviation, of those features are used to model certain aspects of the artist’s brushstrokes. For capturing the local brushstroke texture, we first compute the wavelet transform to the image. A spatial model, the 2-D hidden Markov model, is used to model the texture features of each subimage. The methods have shown to be able to distinguish van Gogh paintings and non van Gogh paintings to a great extent. The techniques can provide clues for the dating of van Gogh paintings. A comparison of the van Gogh paintings, Monticelli’s paintings, and paintings by contemporary artists provides insights on their similarities and differences. The analysis has provided numerical statistics for further studying these and other paintings.

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11:51AM Q3.00002 Prime-Time Science: The Beginning of a Beautiful Friendship? **JENNIFER OUELLETTE, National Academy of Sciences — The portrayal of science has often posed a challenge to Hollywood. Though it has provided some of the compelling storylines, the many complexities of science (and scientists) have confounded even the most talented writer or director, pitting creative license against scientific accuracy again and again. Likewise, the scientific community has struggled to find a conduit through which it can communicate its story to the general public on a mass scale. To bridge this gap, the National Academy of Sciences has partnered with leading Hollywood professionals to launch The Science and Entertainment Exchange; its mission is to connect entertainment industry professionals with top scientists from across the country to foster creative collaborations. The timing has never been better: there is a plethora of network TV shows currently on the air with science-based themes and plot lines, and a renewed interest – even with science fiction films and TV – in coming up with more plausible futuristic scenarios. Working together, the two communities can create a “win-win” synergy between accurate science and engaging entertainment.**

12:27PM Q3.00003 Hollywood Science: Good for Hollywood, Bad for Science? **SIDDNEY PERKOWITZ, Emory University — Like it or not, most science depicted in feature films is in the form of science fiction. This isn’t likely to change any time soon, if only because science fiction films are huge moneymakers for Hollywood. But beyond that, these films are a powerful cultural force. They reach millions as they shed light on current scientific issues and stimulate public interest.**

In this talk, based on my book _Hollywood Science_ [1], I’ll show examples of good and bad screen treatments of science, scientists, and their impact on society. I’ll also discuss efforts to improve how science is treated in film and ways to use even bad movie science to convey real science.

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1:03PM Q3.00004 The Physics of the Blues, J. MURRAY GIBSON, Argonne National Laboratory — In looking at the commonalities between music and science, one sees that the musician’s palette is based on the principles of physics. The pitch of a musical note is determined by the frequency of the sound wave. The scales that musicians use to create and play music can be viewed as a set of rules. What makes music interesting is how musicians develop those rules and create ambiguity with them. I will discuss the evolution of Western musical scales in this context. As a particular example, “Blue” notes are very harmonic notes that are missing from the equal temperament scale. The techniques of piano blues and jazz represent the melding of African and Western music into something totally new and exciting. Live keyboard demonstrations will be used. Beyond any redeeming entertainment value the talk will emphasize the serious connections between science and art in music. Nevertheless tips will be accepted.

1:39PM Q3.00005 Joys and Pains in Making a Science Movie1, IVAN SCHULLER, UCSD — This talk will describe the joys and pains in making a multiple award winning science movie: “When Things Get Small.” We found that in order to reach a wide public of non-experts, the best approach is to develop a collaboration between a scientist and a TV producer. In order to keep scientific accuracy and at the same time maintain public interest it is crucial to keep the message well defined and crisp and not dwell on too many details. The creative process, coming from these two different cultures, makes this a very rewarding experience. However, there are also “pains” associated with it which will be described. Movie available at http://fischuller.ucsd.edu/movies/movies.php or http://uctv.tv/getsmall/ movie was produced in collaboration with R. Wargo and UC-TV(http://www.ucsd.tv/getsmall/) and had the contribution from many other movie professionals.

Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q4 DPOLY GSNP: Polymer Surface Instabilities 306/307

11:15AM Q4.00001 Elastic instabilities in rubber, ALAN GENT, University of Akron — Materials that undergo large elastic deformations can exhibit novel instabilities. Several examples are described: development of an aneurysm on inflating a rubber tube; non-uniform stretching on inflating a spherical balloon; formation of internal cracks in rubber blocks at a critical level of triaxial tension or when supersaturated with a dissolved gas; surface wrinkling of a block at a critical amount of compression; debonding or fracture of constrained films on swelling, and formation of “knots” on twisting stretched cylindrical rods. These various deformations are analyzed in terms of a simple strain energy function, using Rivlin’s theory of large elastic deformations, and the results are compared with experimental measurements of the onset of unstable states. Such comparisons provide new tests of Rivlin’s theory and, at least in principle, critical tests of proposed strain energy functions for rubber. Moreover the onset of highly non-uniform deformations has serious implications for the fatigue life and fracture resistance of rubber components.

References:

11:51AM Q4.00002 Creasing instability of solvent-swelled polymer films, RYAN HAYWARD, University of Massachusetts, Amherst — A thin layer of polymer bound to a rigid substrate develops compressive stresses when it is swelled by solvent, due to the constraint against lateral expansion imposed by the substrate. For sufficiently large stresses, the surface becomes unstable to a buckling mode in which tightly-folded “creases” form on the surface to relieve compressive stress. While this instability has been known in practice for more than a century, it remains poorly characterized and incompletely understood. I will describe experiments on model systems of surface-attached hydrogels to characterize the onset and growth mechanisms of creases, as well as methods that allow control of crease formation in both space and time. In addition to the implications that this instability has for any type of polymeric coating undergoing swelling, it also provides an opportunity to create surfaces with switchable topography and chemistry.

12:27PM Q4.00003 The macroscopic delamination of thin films from elastic substrates, PEDRO REIS, Massachusetts Institute of Technology — The wrinkling and delamination of stiff thin films adhered to a polymer substrate have important applications in “flexible electronics.” The resulting periodic structures, when used for circuity, have remarkable mechanical properties since stretching or twisting of the substrate is mostly accommodated through bending of the film, which minimizes fatigue or fracture. To date, applications in this context have used patterning of the substrate-film adhesion energy to produce a controlled array of delamination “blisters.” However, even in the absence of such patterning, blisters have a characteristic size. We use macroscopic experiments to study what sets the dimensions of these blisters in terms of the material properties, which we explain using a combination of scaling and analytical methods. This points to a novel method for determining the interfacial toughness. Finally, we suggest a number of design guidelines for the thin films used in flexible electronic applications.

1:03PM Q4.00004 Elastic Instability and Pattern Formation in Confined Soft Elastomeric Films, ANIMANGSU GHATAK, Department of Chemical Engineering, IIT Kanpur — When a rigid flat object or a flexible plate is removed from a thin soft film, instability patterns appear at the interface in the form of bubbles or fingers. The wavelengths of these instabilities are independent of all material and geometrical properties of the system except the thickness of the film. These observations contrast the classical Saffman-Taylor type instability in which the instability pattern depends on the viscous and surface tension forces in addition to the thickness of the liquid film. In the case of elastic instability of the kind described here, the wavelength depends on the material properties of the films only when soft films of different elastic properties are separated from each other. In the later case, a co-operative instability mode develops, which is a non-linear function of the thicknesses and the elastic moduli of both the films. In contrast to the wavelengths of these instabilities, their amplitudes are strong functions of several material and geometric properties of the system. These problems can be analyzed using regular perturbation technique to obtain the excess deformations of the film over and above the base quantities. Furthermore, by estimating the excess energy of the system, it can be shown that instability develops when the films are critically confined. This point can be illustrated by pre-stretching the film or simply by adjusting the contact width between the film and the plate. The instabilities that develop at the interface are critical to understanding adhesion and friction of soft thin films as they act like nucleated interfacial cracks. We performed a simple experiment, in which a flat rigid glass prism is sheared off a soft elastomeric film. At a given tangential force, the prism starts to slide on the elastomeric film accompanied with the formation of bubbles at the interface due to elastic instability. These bubbles, the lateral dimensions of which are comparable to the thickness of the film, move across the interface with speeds 1000 times faster than the overall sliding speed of the prism. The process continues till the critical condition for fracture is reached. These studies may shed some light on the fast dynamics of shear crack propagation in other systems.

1:39PM Q4.00005 Micro-Origami: Elastic Instability of Polymer Films, PASCAL DAMMAN, Université de Mons-Hainaut — Upon compression, thin (rigid) elastic membranes supported on a soft elastic solid spontaneously deviate from their flat geometry by forming regular wrinkles. How can we control the wavelength and the symmetry of the wrinkle patterns? What is the influence of defects? Why should we observe focalisation of deformation in folds for large strains? During my talk, I will review our approaches to tackle these questions.

1Work supported by NSF, UCSD and private sources.
Wednesday, March 18, 2009 11:15AM - 2:15PM –
Session Q5 FIAP: Plasmonics in Future Electronics 401/402

11:15AM Q5.00001 A Technique for Nanoscale Plasmonic Imaging via Photoemission . DANIEL S. PICKARD, Department of Electrical Engineering, National University of Singapore — The scientific community is witnessing increased research activity on Surface Plasmon Polaritons (SPPs). The potential applications of SPPs and plasmonic structures based on their control and manipulation are truly multi-disciplinary, spanning high speed nano-scale interconnects, meta-materials, chemical and biological sensing, sub-wavelength optics and waveguides, near-field optical trapping, high-density data storage, and the enhancement of non-linear effects. Measurement of the localized optical field intensity is a critical component in validating physical models and characterizing plasmonic structures. The dominant technique employed for this task is the Scanning Near-Field Optical Microscope (SNOM) or Photon Scanning Tunneling Microscope (PSTM), whose contrast mechanism is based on measuring light scattered from the near-field with a probe. These techniques can provide high resolution images of the localized fields, but they are slow. Furthermore, tip-sample interactions can perturb the fields, yielding ambiguity between electric and magnetic fields and frustrating attempts at accurate optical characterization. One way to facilitate the advance of plasmonics is to develop new techniques for imaging and characterizing SPP behavior on the nanoscale. Recent efforts employing photoemission to reveal the localized fields have demonstrated that this technique can provide both high spatial (∼10nm) and temporal (fs) resolution when combined with a Photoelectron Emission Microscope (PEEM)[1-3]. The PEEM does not require a probe so the fields can be imaged without perturbation. It also provides a parallel image of the full field, so acquisition times are fast. We are expanding the capabilities of the PEEM to exploit a novel contrast mechanism which will broaden the spectrum of plasmonic devices observable. We present our experimental efforts in this area, detail the underlying physics of the contrast mechanism and discuss how it can be controlled to enable unique spatial and temporal information on the propagation of SPPs within plasmonic structures.


11:51AM Q5.00002 Ultrafast and Quantum Nanoplasmonics: SPASER and Control . MARK I. STOCKMAN, Department of Physics and Astronomy, Georgia State University — Nanoplasmonics is presently experiencing a period of unprecedented growth and has numerous applications. These include sensing and detection of minute amount of chemical and biological objects for medicine and defense [1], near-field scanning optical microscopy [2], immunological tests, labels for biomedical research, nanoantennas for efficient coupling of light to semiconductor devices, etc. Nanoplasmonics still greatly needs active elements to generate optical energy on the nanoscale and serve as amplifiers. We have proposed a quantum nanoplasmonic generator and amplifier of the local optical fields, SPASER [surface plasmon amplification by stimulated emission of radiation]. A SPASER is analogous to laser except that light (photons) is replaced by local optical fields (surface plasmons). This is responsible for the principal difference: laser cavity must support photonic modes and its size is on order or much greater than the optical wavelength, cf. [6]. In contrast, the surface plasmons in the spaser are purely electric oscillations whose localization size is nanometric. SPASER will transform nanoplasmonics the same way as the laser transformed optics. In particular nanoplasmonic processors working at THz operation rates will become possible. Another important area is the active control of nanoplasmonic phenomena. One approach to it is coherent control, where a shaped optical pulse dynamically, on the femtosecond scale controls the nanoscale distribution of local fields [7-12].

References

12:27PM Q5.00003 Magnetic Light Emitters: Plasmon-enhanced Magnetic Dipole Transitions . RASHID ZIA, Brown University — Over the past decade, advances in both negative index metamaterials and resonant optical antennas have challenged traditional assumptions about light-matter interactions. While metamaterials research has shown that metallic structures can be engineered to support strong optical frequency magnetic resonances, resonant optical antennas have been designed to amplify and re-direct the emission from electric dipole emitters. In this talk, we explore the intersection of these distinct fields and investigate how resonant optical effects may be used to challenge the electric dipole approximation. Specifically, we will show how Purcell effects may be used to enhance the natural optical frequency magnetic dipole transitions in Lanthanide ions. We will present experimental and numerical results that demonstrate enhanced magnetic dipole emission from trivalent Europium ions near metallic films and nanoparticle composites. We will explore how the varying symmetries of electric and magnetic dipoles can be used to characterize and optimize magnetic light emission. Finally, we will discuss the implications of enhancing and controlling higher-order optical transitions for optical spectroscopy and photonic devices.

1:03PM Q5.00004 Plasmonic nano-circuitry . SERGEY BOZHEVOLNYI, University of Southern Denmark — Photonic components are superior to electronic ones in terms of operational bandwidth but suffer from the diffraction limit that constitutes a major problem on the way towards miniaturization and high density integration of optical circuits. The degree of light confinement in dielectric structures, including those based on the photonic band-gap effect, is fundamentally limited by the light wavelength in the dielectric used. The main approach to circumvent this problem is to take advantage of hybrid nature of surface plasmons (SPs) whose subwavelength confinement is achieved due to very short (nm-long) penetration of light in metals. After briefly reviewing various SP guiding configuration the results of our investigations of subwavelength photonic components utilizing SP modes propagating along channels cut into gold films are overviewed [Nature 440, 508 (2006); Nano Lett. 7, 880 (2007)], demonstrating first examples of ultracompact photonic components that pave the way for a new class of integrated optical circuits [Physics Today, May 2008, pp.44-50]. Recent results on the SP guiding along gold wedges at telecom wavelengths are also presented [Opt. Express 16, 5252 (2008)].
Field enhancement by Plasmonic Nanostructures

JOHN G. RADZILOWICZ, Carnegie Science Center — The late Carl Sagan opined that somehow we have managed to create a global civilization dependant on science and technology in which almost no one understands science and technology. This is an unacceptable recipe for disaster with social, political and financial implications for the future of scientific research. And so, like it or not, popular science communication, more than ever before, is an important and necessary part of the scientific enterprise. Public outreach programs, media interviews, and popular articles have become required parts of the scientist’s professional repertoire. But, what does it take to be a good science communicator? What is needed to develop and deliver meaningful public outreach programs? How do you handle non-technical presentations? And, what help is available in developing the necessary skills for good popular science communication? This presentation will look at the essential components of effective science communication aimed at a broad public audience. The components of successful science communication in programs, presentations and articles will be discussed. Specific attention will be given to how university-museum partnerships can expand the reach and enhance the quality of public outreach programs.

11:15AM Q6.00001 So, You Want to be a Science Communicator? , JOHN G. RADZILOWICZ, Carnegie Science Center — The late Carl Sagan opined that somehow we have managed to create a global civilization dependant on science and technology in which almost no one understands science and technology. This is an unacceptable recipe for disaster with social, political and financial implications for the future of scientific research. And so, like it or not, popular science communication, more than ever before, is an important and necessary part of the scientific enterprise. Public outreach programs, media interviews, and popular articles have become required parts of the scientist’s professional repertoire. But, what does it take to be a good science communicator? What is needed to develop and deliver meaningful public outreach programs? How do you handle non-technical presentations? And, what help is available in developing the necessary skills for good popular science communication? This presentation will look at the essential components of effective science communication aimed at a broad public audience. The components of successful science communication in programs, presentations and articles will be discussed. Specific attention will be given to how university-museum partnerships can expand the reach and enhance the quality of public outreach programs.

11:15AM Q6.00002 Public Outreach for the International Year of Astronomy Through Faculty and Science Center Partnerships1 , ANDREW ZENTNER, University of Pittsburgh — The International Year of Astronomy 2009 provides an opportunity to jump-start public education and outreach programs and to engage the community in a fascinating field. In my talk I will discuss a diverse program of education and outreach designed and implemented as a collaborative effort between the Astronomy faculty at the University of Pittsburgh and the Carnegie Science Center. I will highlight some of the unique benefits of such a partnership and some of the unique events such a partnership enables.

12:27PM Q6.00003 Public Education and Outreach Through Full-Dome Video Technology1 , JOHN POLLOCK, Duquesne University — My long-term goal is to enhance public understanding of complex systems that can be best demonstrated through richly detailed computer graphic animation displayed with full-dome video technology. My current focus is on health science advances that focus on regenerative medicine, which helps the body heal itself. Such topics facilitate science learning and health literacy. My team develops multi-media presentations that bring the scientific and medical advances to the public through immersive high-definition video animation. Implicit in treating the topics of regenerative medicine will be the need to address stem cell biology. The topics are clarified and presented from a platform of facts and balanced ethical consideration. The production process includes communicating scientific information about the excitement and importance of stem cell research. Principles of function are emphasized over specific facts or terminology by focusing on a limited, but fundamental set of concepts. To achieve this, visually rich, biologically accurate 3D computer graphic environments are created to illustrate the cells, tissues and organs of interest. A suite of films are produced, and evaluated in pre-post-surveys assessing attitudes, knowledge and learning. Each film uses engaging interactive demonstrations to illustrate biological functions, the things that go wrong due to disease and disability, and the remedy provided by regenerative medicine. While the images are rich and detailed, the language is accessible and appropriate to the audience. The digital, high-definition video is also re-edited for presentation in other “flat screen” formats, increasing our distribution potential. Show content is also presented in an interactive web space (www.sepa.duq.edu) with complementing teacher resource guides and student workbooks and companion video games.

1:03PM Q6.00004 A New Approach to A Science Magnet School - Classroom and Museum Integration , SAMUEL FRANKLIN, Pittsburgh Science and Technology Academy — The Pittsburgh Science & Technology Academy is a place where any student with an interest in science, technology, engineering or math can develop skills for a career in life sciences, environmental sciences, computing, or engineering. The Academy isn’t just a new school. It’s a new way to think about school. The curriculum is tailored to students who have a passion for science, technology, engineering or math. The environment is one of extraordinary support for students, parents, and faculty. And the Academy exists to provide opportunities, every day, for students to Dream. Discover. Design. That is, Academy students set goals and generate ideas, research and discover answers, and design real solutions for the kinds of real-world problems that they’ll face after graduation. The Academy prepares students for their future, whether they go on to higher education or immediate employment. This talk will explain the unique features of the Pittsburgh Science & Technology Academy, lessons learned from its two-year design process, and the role that the Carnegie Museums have played and will continue to play as the school grows.

1:39PM Q6.00005 Fractured Physics and the Great Color Caper: Large Scale Physics Outreach , MIKE HENNESSY, Carnegie Science Center — No abstract available.

Wednesday, March 18, 2009 11:15AM - 2:15PM –
12:27PM Q7.0003 Fast, continuous recirculation of germinal center B cell populations enhances robustness of immune response towards varying pathogens, MICHAEL DEEM, Rice University — The immune system normally protects the human host against death by infection. I will introduce a physical theory of the evolutionary dynamics that occurs in the antibody-mediated and T cell-mediated immune responses. The theory will be used to provide a mechanism for original antigenic sin, wherein an initial exposure to antigen can degrade the response of the immune system upon subsequent exposure to related, but different, antigens. A new order parameter to characterize antigenic distance will be introduced from the theory. This order parameter predicts effectiveness of the influenza vaccine more reliably than do results from animal model studies currently used by world health authorities. I will discuss how this order parameter might be a valuable new tool for making vaccine-related public health policy decisions. Next, I will briefly discuss dengue fever. Infection with, or vaccination against, one of the four serotypes of dengue fever typically increases susceptibility to dengue hemorrhagic fever from one of the other three serotypes. I will present a physical theory of this immunodominance and use this theory to quantify the predicted mitigation of immunodominance in a novel formulation of the dengue vaccine.

1:03PM Q7.0004 Fish Immunology, STEPHEN QUAKE, Stanford Univ — No abstract available.

1:39PM Q7.0005 Genetic Circuit Architectures Underlying Cell Fate Choices for Immunity, AARON DINNER, The University of Chicago — Antigen stimulated B cells follow an unusual developmental trajectory that transiently passes through a germinal center state, which promotes receptor affinity maturation and immunoglobulin class switching, before terminally differentiating into antibody secreting plasma cells. It was found that graded expression of the transcription factor IRF-4 regulates cell fate, but the relationship between antigen receptor signaling, the network of interactions with IRF-4, and cell fate was not known. This talk describes models that link ligand-receptor avidity with cell fate. The models have been validated experimentally by directly varying the levels and kinetics of IRF-4 accumulation. Furthermore, signaling through the antigen receptor is demonstrated to control the expression of IRF-4 and in turn the frequency of B cells that undergo class switching before differentiating into plasma cells. These findings provide an explanation for experiments that measure B cell numbers in transgenic mice. The architecture of our regulatory circuit provides a general mechanism for quantitative variations in a signal to be translated into a binary cell-fate choice involving transient expression of one of the two developmental fates. In collaboration with Arvye Warmflash, Ying Li, Roger Sciammas, and Harinder Singh, The University of Chicago.

Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q8 GMAG: Quantum Spin Dynamics and Relaxation in Molecular Magnets

11:15AM Q8.00001 Coherent Manipulation and Decoherence of S=10 Single-Molecule Magnets, SUSUMU TAKAHASHI, University of California Santa Barbara — A single crystal of high-spin single-molecule magnets (SMMs) is an attractive testbed for quantum science and technologies. High-spin SMMs are suitable for applications to dense quantum memory and computing devices. Because SMM clusters are identical and interact weakly, the ensemble properties of single crystals of SMMs reflect the properties of a single cluster. However coherent manipulation of high-spin SMM crystals has never been demonstrated due to strong spin decoherence. For spins in the solid state, an interaction with fluctuations of surrounding spin bath is a major source of spin decoherence. One approach to reduce spin bath fluctuations is to bring the spin bath into a well-known quantum state that exhibits little or no fluctuations. A prime example is the approach of using a fully polarized spin bath. In diamond, spin decoherence has been quenched using high-frequency pulsed electron paramagnetic resonance (EPR) [1]. We present coherent manipulation and decoherence of a single-crystal of S=10 Fe8 SMMs. Through pulsed polarization in Fe8 SMMs at 4.6 T and 1.3 K, we demonstrate that spin decoherence is significantly suppressed to extend the spin decoherence time (T2) up to 700 ns [2]. Investigation of temperature dependence of spin relaxation times reveals the nature of spin decoherence. This work is collaboration with J. van Tol, C. C. Beedle, D. N. Hendrickson, L.-C. Brunel, and M. S. Sherwin.


11:51AM Q8.00002 The Role of Antisymmetric Exchange on the Quantum Interference between States of Different Spin Length in a dimeric Molecular Nanomagnet, ENRIQUE DEL BARCO, University of Central Florida — We report direct evidence of quantum oscillations of the total spin length of a dimeric molecular nanomagnet through the observation of the splitting of NMR signals originating from EPR line broadening and tunneling. The EPR line broadening is given by the spin Hamiltonian for a single Mn12 wheel which behaves as a weak ferromagnetic exchange-coupled molecular dimer: each half of the molecule acts as a single-molecule magnet (SMM), while the weak coupling between the two halves gives rise to an additional internal spin degree of freedom within the molecule, namely that its total spin may fluctuate. This extra degree of freedom accounts for several magnetization tunneling resonances that cannot be explained within the usual giant spin approximation. More importantly, the observation of quantum interference provides unambiguous evidence for quantum mechanical superposition involving entangled states of both halves of the wheel. Magnetization results obtained in two other versions of this compound, in which the ligands have been modified, show that slight variations of the relative distance between the Mn ions determine whether the molecule behaves as a rigid magnetic unit of spin S = 7 or as two exchange-coupled halves of spin S = 7/2. We analyze the effect of the Dzyaloshinskii-Moriya anti-symmetric exchange interaction in a molecule with a centre of inversion symmetry and propose a formal model to account for the observed broken degeneracy that preserves the molecular inversion symmetry.
12:27PM Q8.00003 Spin dynamics in the single molecule magnet Ni₈ under microwave irradiation¹. GREGOIRE DE LOUBENS². Department of Physics, New York University — Quantum mechanical effects such as quantum tunneling of magnetization (QTM) and quantum phase interference have been intensively studied in single molecule magnets (SMMs). These materials have also been suggested as candidates for qubits and are promising for molecular spintronics. Understanding decoherence and energy relaxation mechanisms in SMMs is then both of fundamental interest and important for the use of SMMs in applications. Interestingly, the single-spin relaxation rate due to direct process of a SMM embedded in an elastic medium can be derived without any unknown coupling constant [1]. Moreover, nontrivial relaxation mechanisms are expected from collective effects in SMM single crystals, such as phonon superradiance or phonon bottleneck. In order to investigate the spin relaxation between the two lowest lying spin-states of the S = 4 single molecule magnet Ni₈, we have developed an integrated sensor that combines a microstrip resonator and micro-Hall effect magnetometer on a chip [2]. This sensor enables both real time studies of magnetization dynamics under pulse irradiation as well as simultaneous measurements of the absorbed power and magnetization changes under continuous microwave irradiation. The latter technique permits the study of small deviations from equilibrium under steady state conditions, i.e. small amplitude cw microwave irradiation. This has been used to determine the energy relaxation rate of a Ni₈ single crystal as a function of temperature at two frequencies, 10 and 27.8 GHz. A strong temperature dependence is observed below 1.5 K, which is not consistent with a direct spin-phonon relaxation process. The data instead suggest that the spin relaxation is dominated by a phonon bottleneck at low temperatures and occurs by an Orbach process involving excited spin-levels at higher temperatures [3]. Experimental results will be compared with detailed calculations of the relaxation rate using the density matrix equation with the relaxation terms in the universal form.


¹This research was done in collaboration with A. D. Kent, D. A. Garanin, C. C. Beedle and D. N. Hendrickson and supported by NSF-DMR-0506946.
²Present address: SPEC, CEA Saclay, France

1:03PM Q8.00004 Multiphoton Coherent Manipulation in Large Spin Qubits¹. IRINEL CHIORESCU, Florida State University, Department of Physics and National High Magnetic Field Laboratory — Manipulation of quantum information allows certain algorithms to be performed at unparalleled speeds. Photons are an ideal choice to manipulate qubits as they interact with quantum systems in predictable ways. They provide a mechanism for measuring and controlling qubits located far apart. This has enabled new advances in quantum communication and quantum computing. Photons and qubits can also be manipulated with other methods such as atomic interaction. This talk will present multiphoton methods, which can be applied to qubits with more than 10⁶ spins. These multiphoton methods can be used to control quantum systems in a large spin qubit.

1:39PM Q8.00005 Understanding electron and nuclear spin dynamics in Cr₅⁺ doped K₂NbO₅¹. SARITHA NELLUTLA, North Carolina State University — Chromium(V) doped in the diamagnetic host potassium niobate, a simple spin S = 1/2, I = 0 system, has been proposed as an alternative standard for field calibration and q-standard for high-field EPR [1]. This system constitutes a dilute two-level model relevant for use as an electron spin qubit [2] and as such coherent electron spin manipulation at X-band (~9.5 GHz) was observed over a wide range temperature. Rabi oscillations are observed for the first time in a spin system based on transition metal oxides up to room temperature. At 4 K, a Rabi frequency Ω₅ of 20 MHz together with the phase coherence relaxation (spin-spin relaxation) time, T₂ of ~10 μs results in the single qubit figure of merit Q₅M = Ω₅T₂/π as about 500, showing that a diluted ensemble of Cr⁵⁺(S = 1/2) doped K₂NbO₅ is a potential candidate for solid-state quantum information processing. Also, the field and temperature dependence of the T₁ (spin-lattice relaxation) and T₂ times was investigated [3] for a further understanding of the relaxation mechanisms governing the phase decoherence in this system. These studies show that the coupling of the electron spin with the neighboring ⁴⁰K nuclei (I = 3/2) is one of the prominent T₂ mechanisms. The hyperfine and quadrupole interactions with ⁴⁰K nuclei was resolved by using the high-frequency (240 GHz) pulsed nuclear electron double resonance (ENDOR) technique.

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Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q9 GSNP: Focus Session: Dynamics of Glassy Systems 303

11:15AM Q9.00001 Geometric interpretation of pre-vitrification in hard sphere glasses, MATTHIEU WYART, School of Engineering and Applied Sciences, Harvard University — I will derive a geometric condition for the stability of hard sphere configurations, and I will show empirically that this condition is saturated in the glass phase. The marginal stability observed explains the presence of slow modes in the short term dynamics of the glass, and supports a microscopic interpretation for the rapid initial rise of the viscosity, or pre-vitrification, when the packing fraction increases. This observation also suggests a possible cause for the collective nature of the structural relaxation near the glass transition.
11:51AM Q9.00002 Aging of a Colloidal Suspension of Thermosensitive Particles, KYAW WIN, GREGORY MCKENNA, Chemical Engineering, Texas Tech University, TX 79409, TETSUHARU NARITA, FRANCOIS LEQUEUX, Laboratory PPM, UPMC-ESPCI-CNRS UMR7615, SRINIVAS PULLELA, ZHENGDONG CHENG, Chemical Engineering, Texas A&M University, TX 77843 — We have studied the aging behavior of a concentrated suspension of thermosensitive particles (PNIPAM). We found that the characteristic time of the dynamics of the system as a function of waiting time obeys the usual power law with exponent $\sim 1$ both after shear melting the system and after a jump in temperature which is equivalent to a jump in concentration. We also report for the first time the observation of an extreme asymmetry of approach in the aging behavior with respect to down jump and up jump in temperature. While an asymmetry effect is already known in conventional glass formers such as polymers and small molecule liquids, it is both much more pronounced in the colloidal PNIPAM suspension and of a fundamentally different character.

12:03PM Q9.00003 Rejuvenation and memory in a 2D colloidal glass, JENNIFER M. LYNCH, Physics Dept., Emory University, ZEXIN ZHANG, PETER YUNKER, ARJUN G. YODH, Physics Dept., University of Pennsylvania, ERIC R. WEEKS, Physics Dept., Emory University — We work with a 2D colloidal system that has a glass transition and use this system to experimentally observe memory and rejuvenation effects as the sample ages. In particular, we study a system of colloidal particles made of thermosensitive poly(N-isopropylacrylamide) (NIPA) polymer. The sample is confined in a narrow quasi-2D gap between parallel glass plates, which allows easy observation and rapid temperature response. Lowering temperature increases the size of the colloidal particles, which can induce the glassy state due to the crowding of the particles. When our colloidal sample is quenched into the glassy state, particle motion slows over time; this is aging. In molecular glasses, prior experiments studied how aging is modified when the temperature is changed while the sample ages, finding that aging at a first temperature $T_1$ and aging at a later time with second temperature $T_2$ are mostly independent. “Memory” relates to the case $T_1 < T_2$ and “rejuvenation” to the opposite case. Our colloidal system allows us to observe both of these effects.

12:15PM Q9.00004 A continuous time random walk description of the hopping dynamics in an aging polymer glass, MYA WARREN, JOERG ROTTLER, University of British Columbia — Due to the non-equilibrium nature of the glassy state, structural relaxation becomes increasingly sluggish with the wait time $t_w$ since vitrification. As a result, dynamical correlation functions age, and often obey a simple rescaling with $t_w$: $C(t, t-w) = C_0(t) + C_{\text{vpc}}(t/t_w)$. It has recently been shown that, to first order, scaling also applies to the distributions of local correlations and displacements (the van Hove function). In this study, we use molecular dynamics simulations to measure the statistics of the discontinuous hopping events that characterize structural relaxations during aging. This allows us to map the particle dynamics onto a continuous time random walk, which successfully reproduces the entire distribution of displacements. Our results bear a striking resemblance to the popular trap model of aging. We find that the hop time distribution takes the form of a power law which is independent of $t_w$, whereas the time to the first hop shifts to longer times with $t_w$. This two-timescale behavior explains not only the scaling of the distribution functions for times $t \sim t_w$, but also small deviations from perfect scaling that have been observed at longer times.

12:27PM Q9.00005 The Defect Diffusion Model and Isochoric Energy and Isobaric Enthalpy for Glass Formers, MICHAEL SHLESINGER, Physics Department, U.S. Naval Academy, Annapolis, MD 21402-5026 and Office of Naval Research, Code 30, 875 N. Randolph St., Arlington VA 22203, JOHN BENDLER, Department of Chemistry, South Dakota School of Mines, Rapid City, SD 57701 and Physics Department, U.S. Naval Academy, Annapolis, MD 21402-5026 — The defect diffusion model produces stretched exponential relaxation, in supercooled liquids, through the sub-diffusive motion of defects. The aggregation of the defects produces a Vogel-Fulcher type law for the divergence of the time scale at a critical temperature. The model is employed to calculate the ratio of the apparent isochoric activation energy to the isobaric activation enthalpy, $E_{I}/H_{I}$ or $E_{V}/E_{P}$. This ratio measures the relative sensitivity of kinetic processes to changes in volume and temperature respectively. This ratio equation is tested using dielectric relaxation data for poly(vinyl acetate), viscosity data for glycerol and ionic conductivity data for poly(propylene glycol) containing LiCF$_3$SO$_3$. Good agreement between theory and experiment is found using model parameters previously published.

12:39PM Q9.00006 Fluctuations in the relaxation of a strong glass, AZITA PARSAEIAN, HORACIO E. CASTILLO, Department of Physics and Astronomy, Ohio University, KATHARINA VOLLMAYR-LEE, Department of Physics and Astronomy, Bucknell University — We present results of molecular dynamics simulations of amorphous silica, carried out by using the BKS inter-atomic potential. We quantify the evolution of fluctuations by studying the probability distributions of local observables such as individual particle displacements $\Delta r$ and local coarse grained intermediate scattering functions $C_{\vec{q}}$. We test for universality by comparing the probability distributions with those in small molecule glasses and in polymer glasses.

12:51PM Q9.00007 A percolation model for dynamics in glass-forming materials, GREGG LOIS, JERZY BLAWDZIEWICZ, COREY O’HERN, Yale University — We characterize the glass to liquid transition as a percolation of mobile regions in configuration space. We find that many hallmarks of glassy dynamics, for example stretched-exponential response functions and a diverging structural relaxation time, result from critical properties of mean-field percolation. Specific predictions of the percolation model include the range of possible stretching exponents $1/3 \leq \beta \leq 1$ and the functional dependence of the alpha relaxation time and stretching exponent on temperature, density, wave number, and entropy.

1:03PM Q9.00008 Finite Temperature Simulations of Glassy Models with Patchwork Dynamics, CREIGHTON THOMAS, ALAN MIDDLETON, Syracuse University — We present simulation results on aging effects in the late time dynamics of two glassy models: the Edwards-Anderson Ising spin glass and a disordered lattice dimer model. As these models have glassy dynamics, direct simulations take prohibitively long times. We use patchwork dynamics, in which we replace local Monte Carlo updates with efficient exact finite temperature equilibration of subsystems, or patches. We scale the simulation data and find a collapse to relate the dynamics for different patch sizes, with larger patches evolving the system more rapidly. We investigate the use of this technique to study rejuvenation and memory effects.

1:15PM Q9.00009 Connecting microscopic and phenomenological approaches to glassy dynamics, MALCOLM KENNEDT, Simon Fraser University, MATTHEW DOWNTON, Technische Universität Berlin — Kinetically constrained spin models are known to exhibit dynamical behavior mimicking that of glass forming systems. They are often understood as coarse-grained models of glass formers, in terms of some “mobility” field. The identity of this “mobility” field has remained elusive due to the lack of coarse-graining procedures to obtain these models from a more microscopic point of view. Here we exhibit a scheme to map the dynamics of a two-dimensional soft disc glass former obtained from Molecular Dynamics simulations onto a kinetically constrained spin model, providing an attempt at bridging these two approaches.
interaction, whereas the underlying mechanism of multiferroicity in frustrated manganites \( R_2 \) in the magnetoelectric coupling in YMn
induced polarization reverses at the temperature where the polarization changes its sign. The temperature dependence of spin correlation along the propagating
onset temperature
2 temperature-dependent spin ordering of multiferroic YMn
1 the number of rigid structures that a system of N particles can form grows exponentially with N. Stabilizing any one structure over all others is thus a challenging problem. We consider a system of N spherical colloidal particles that cannot deform or overlap, and which exhibit a short-range attractive force. We present a method, using graph theory and geometry, that solves for all possible rigid packings of N particles - the resultant set of packings is provably complete. We then present a mechanism that is capable of stabilizing any one structure over all others (in the zero temperature limit), and which is experimentally realizable - thereby, potentially allowing us to direct the self-assembly of a desired structure. We compare to preliminary experimental results.

Aberdam et al., Surface Science 3
evident but with less consistent order. The 2-D lattice constant parameters in (0001) plane are consistent with previous literature values for pure YMnO
sharp growth fronts initiated at the free surface and at the interface with the substrate. For the free surface, the growth velocity is constant in time and has the
domain structure below and above the Curie temperature of \( \sim T_{C-L} \) of ferroelectricity, the handedness of cycloidal spin spirals exists, but vanishes above \( C \). The spin handedness perpendicular to the
domains are visible up from 500˚C to \( \sim 630 \) ˚C. The domain contrast in LEEM was lower upon cooling and we are exploring several
patterns were obtained for all samples with the sharpest LEED contrast near T
100 nm to \( 5 \) µm. The domains are evident from \( 500 ^\circ C \) to ~900 \(^\circ C\), giving possible evidence for the expected 180° ferroelectric domain structure below and above the Curie temperature of \( \sim 630 \) °C. The domain contrast in LEEM was lower upon cooling and we are exploring several
mechanisms for this result. In addition, we observed LEED patterns from ~24 to 1100 °C, with electron energies in the range of 15eV to 50eV. Above 500 °C, 1×1 and 2×2 patterns were obtained for all samples with the sharpest LEED contrast near T \( \sim 1000 ^\circ C\). In some cases a 2×4 surface reconstruction was also evident but with less consistent order. The 2-D lattice constant parameters in (0001) plane are consistent with previous literature values for pure Y MnO (see: Aberdam et al., Surface Science 14, pp.121-140 (1969)).

1:27PM Q9.00010 Glassy Dynamics in Systems of Ellipse-shaped Particles
1. CARL SCHRECK, Yale University, MITCH MAILMAN, BULBUL CHAKRABORTY, Brandeis University, COREY O’HERN, Yale University — Glass-forming materials possess a critical cooling rate \( r^* \); for thermal quench rates \( r > r^* \), these systems form disordered solids; for \( r < r^* \), they form (poly) crystalline materials. We investigate the influence of particle shape (or anisotropic interactions) on the critical cooling rate. In particular, we perform molecular dynamics (MD) simulations of elliptoiodal particles in 2D as a function of aspect ratio of the major to minor axes to optimize the local packing efficiency and the critical cooling rate to improve glass-forming ability. Also, previous mode-coupling theoretical studies have predicted that over a wide range of aspect ratios, the rotational and translational degrees of freedom undergo dynamical arrest at the same temperature. We will perform MD simulations as a function of the cooling rate, packing fraction, and aspect ratio to determine whether novel glass phases also exist in which the rotational and translational degrees of freedom freeze at different temperatures.

1:39PM Q9.00011 Self-Assembly of Spherical Colloidal Particles at Low N
1. NATALIE ARKUS, VINOTHAN MANOHARAN, MICHAEL BRENNER, Harvard University — The number of rigid structures that a system of N particles can form grows exponentially with N. Stabilizing any one structure over all others is thus a challenging problem. We consider a system of N spherical colloidal particles that cannot deform or overlap, and which exhibit a short-range attractive force. We present a method, using graph theory and geometry, that solves for all possible rigid packings of N particles - the resultant set of packings is provably complete. We then present a mechanism that is capable of stabilizing any one structure over all others (in the zero temperature limit), and which is experimentally realizable - thereby, potentially allowing us to direct the self-assembly of a desired structure. We compare to preliminary experimental results.

1:51PM Q9.00012 Aging in the shear-transformation-zone theory of plastic deformation
1. JOERG ROTTLER, University of British Columbia, PHILIPP MAASS, Technische Universitas Ilmenau — Aging phenomena in the plastic response of glassy solids are studied within the theory of shear transformation zones (STZs), which describes the kinetic rearrangement of localized defects in response to external stress. To account for the slow, non-equilibrium dynamics after a quench below the glass transition temperature, two possible models are considered. In the first model, transition rates between the internal states of STZs decrease with time, while in the second model aging occurs due to the relaxation of an effective temperature that determines the number density of STZs and other out-of-equilibrium degrees of freedom. We show that for reasonable choices of parameters, both models capture qualitatively typical aging features seen in computer simulations and experiments on polymer and other soft glasses: (i) Compliance curves measured for different waiting times after the quench can be superimposed when the observation times are rescaled with relaxation times, and (ii) stress-strain curves show a stationary plateau stress independent of waiting time and a peak stress that increases logarithmically with both waiting time and the strain rate.

2:03PM Q9.00013 Stable glass transformation to supercooled liquid via surface-initiated growth front
1. MARK EDIGER, STEPHEN SWALLEN, KATHERINE TRAYNOR, ROBERT MCMAHON, University of Wisconsin-Madison, THOMAS MATES, University of California-Santa Barbara — Recently it has been established that vapor deposition onto substrates at 0.85 Tg can produce high density, high stability, low enthalpy glasses. These glasses may be the most stable ever produced in a laboratory (using the glass formed by cooling the liquid as the reference state). Here we use SIMS to observe the transformation of isotopically layered stable glasses of trisnaphthylbenzene into a liquid during annealing above Tg. In contrast to the predictions of standard models, the observed transformation is spatially heterogeneous. The liquid grows into the stable glass with sharp growth fronts initiated at the free surface and at the interface with the substrate. For the free surface, the growth velocity is constant in time and has the

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11:15AM Q10.00001 Low-energy Electron Microscopy (LEEM) Imaging and Diffraction of Ho1-x Yx MnO3 (0001)
1. M.D. ULRICH, ARO and NCSU, RELJIA VASIC, NCSU, J.T. SADOWSKI, Center for Functional Nanomaterials, BNL, J.E. (JACK) ROWE, NCSU, H.D. ZHOU, C.R. WIEBE, National Magnetic Field Lab, FSU — We have investigated the (0001) surfaces of several hexagonal perovskite alloys Ho1-x Yx MnO3 (x=0-1), by low-energy electron microscopy (LEEM) using both mirror-mode imaging and diffraction (LEED) techniques. We find LEEM structured domains for our (0001) surfaces of single crystals grown by a traveling-solvent-floating zone technique which are likely due to work function variations on a scale of ~100 nm to 5 µm. The domains are visible up from 500 °C to ~900 °C, giving possible evidence for the expected 180° ferroelectric domain structure below and above the Curie temperature of ~630 °C. The domain contrast in LEEM was lower upon cooling and we are exploring several mechanisms for this result. In addition, we observed LEED patterns from ~24 to 1100 °C, with electron energies in the range of 15eV to 50eV. Above 500 °C, 1×1 and 2×2 patterns were obtained for all samples with the sharpest LEED contrast near T ~1000 °C. In some cases a 2×4 surface reconstruction was also evident but with less consistent order. The 2-D lattice constant parameters in (0001) plane are consistent with previous literature values for pure YMnO3 (see: Aberdam et al., Surface Science 14, pp.121-140 (1969)).

11:27AM Q10.00002 Spin Correlation and Magnetically Induced Ferroelectricity in YMnO5
1. J. OKAMOTO, D. J. HUANG, W. B. WU, S. L. CHENG, C. T. CHEN, National Synchrotron Radiation Research Center, Taiwan, C. Y. MOU, National Center for Theoretical Sciences, Taiwan, K. S. CHAO, S. W. HUANG, National Chiao-Tung University, Taiwan, S. PARK, S-W. CHEONG, Rutgers University, USA — There is great interest in understanding the microscopic nature of the coupling between ferroelectricity and magnetic ordering in several multiferroic frustrated manganites \( R MnO_3 \) and \( R Mn_2 O_5 \) (\( R = \) rare earth and Y). For \( R MnO_3 \), the multiferroicity can be understood in terms of the anti- symmetric spin interaction, whereas the underlying mechanism of multiferroicity in \( R Mn_2 O_5 \) remains controversial, because of its structural complexity. We unraveled the temperature-dependent spin ordering of multiferroic YMnO3 by using resonant soft x-ray magnetic scattering at Mn L3 edge. For temperatures below the onset temperature \( T_C \) of ferroelectricity, the handedness of cycloidal spin spirals exists, but vanishes above \( T_C \). The spin handedness perpendicular to the induced polarization reverses at the temperature where the polarization changes its sign. The temperature dependence of spin correlation along the propagating direction of spin spirals resembles the temperature behavior of polarization. These data imply that both symmetric and antisymmetric spin interactions involve in the magnetoelectric coupling in YMnO5.
11:39AM Q10.00003 Magnetic field effects on charge and magnetic structures in a new multiferroic LuFe$_2$O$_4$¹, JINSHENG WEN, GUANGYONG XU, GENDA GU, STEVE SHAPIRO, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA — LuFe$_2$O$_4$ is a new multiferroic where the ferroelectric polarization originates from valence order of Fe$^{2+}$ and Fe$^{3+}$ ions instead of cation displacements. It evolves from two- to three-dimensional charge ordered state upon cooling, and the bulk polarization appears when the charges order three dimensionally. A ferrimagnetic order appears with further cooling. Bulk polarizations and the charge order are both enhanced when the magnetic order occurs, suggesting a strong coupling between the two orders in the system. We have performed neutron scattering measurements on both the charge and magnetic orders under external magnetic fields. We will discuss the field effects and their implications.

¹The work at Brookhaven National Laboratory was supported by the U.S. Department of Energy under contract No. DE-AC02-98CH10886.

11:51AM Q10.00004 Reentrant ferroelectricity and the multiferroic phase diagram of Mn$_{1-x}$Fe$_2$WO$_4$, RAJIT CHAUDHURY, BERND LORENZ, YAQI WANG, YANYI SUN, CHING CHU. TCSUH and Department of Physics, University of Houston, Houston, Texas 77204-5002, USA — Recently MnWO$_4$ has attracted attention because of its multiferroic properties. In MnWO$_4$ the Mn$^{2+}$ ions can be substituted by Fe$^{3+}$ since MnWO$_4$ and FeWO$_4$ are isomorphic. This opens the possibility to tune the magnetic orders by Fe-substitution for a better understanding of the microscopic interactions resulting in the multiferroic properties. We report the discovery of reentrant ferroelectricity in the phase diagram of multiferroic Mn$_{1-x}$Fe$_2$WO$_4$ single crystals. At zero magnetic field (H) the spin-spiral ferroelectric (FE) state is completely suppressed at Fe substitutions (x) exceeding 0.04. For x<0.04 a ferroelectric phase exists in a narrow temperature (T) range at zero magnetic field. This FE phase shows a reentrant behavior at lower T above a critical magnetic field H$_c$(x). The reentrant FE transition is explored by polarization, dielectric constant, and magnetization measurements. The complete multiferroic x-T-H phase diagram of Mn$_{1-x}$Fe$_2$WO$_4$ is derived.

12:03PM Q10.00005 X-ray resonant magnetic scattering study of multiferroic R$\text{MnO}_3 (R=\text{Dy, Ho, Er})$ compounds, A.I. GOLDMAN¹, S. NANDI¹, A. KREYSIG¹, L. TAN¹, J.W. KIM¹, J.Q. YAN¹, M.D. VANNETTE¹, J.C. LANG², D. HASKEL³, T.A. LOGRASSO², R.J. MCQUEENEY¹, ¹Dept. of Physics and Astronomy, Iowa State University, Ames; ²Ames Laboratory US DOE, Ames; ³Advanced Photon Source, Argonne — Element specific x-ray resonant magnetic scattering (XRMS) investigations were undertaken to determine the magnetic structure of multiferroic hexagonal R$\text{MnO}_3$ compounds. In the intermediate temperature phase (ITP) (8-68 K for the Dy$^{3+}$ and 4.5-40 K for Ho$^{3+}$) the moments are aligned and antiferromagnetically correlated in the c direction according to the same magnetic representation $\Gamma_3$. Below the ITP, the Dy$^{3+}$/Ho$^{3+}$ moments order differently and according to the magnetic representations $\Gamma_1$/$\Gamma_2$. The temperature dependence of the observed intensity in the ITP can be modeled assuming the splitting of ground-state doublet/quasi-doublet crystal-field levels of Dy$^{3+}$/Ho$^{3+}$ by the exchange field of Mn$^{2+}$. No resonant signals could be found for Er$^{3+}$ from 2-80 K. Specific magnetic representations can be excluded for the magnetic order of Er$^{3+}$ moments but can not be uniquely determined within the sensitivity of XRMS. — The work supported by U.S. DOE (DE-AC02-07CH11358 and DE-AC02-06CH11357) is acknowledged.

12:15PM Q10.00006 Frequency dependent magneto-dielectric effect in bilayer manganite Pr$_{(Sr_{0.1}Ca_{0.9})_2}$MnO$_7$, BARNALI GHOSH-SAHA, S.N. Bose National Centre for Basic Sciences, D. BHATTACHARYA, Central Glass and Ceramic Institute, S. PATNAIK, Jawaharlal Nehru University, A.K. RAYCHAUDHURI, S. ARUMUGAM — We report novel frequency dependent magneto-dielectric effect and a strong dielectric anomaly near Neel temperature (T$_N$) in a single crystal of bilayer manganite Pr$_{(Sr_{0.1}Ca_{0.9})_2}$MnO$_7$ system. The magneto-dielectric effect measured in a field of 3T shows large frequency dependence and reaches a maximum (∼25%) near T$_N$ at a measurement frequency of 1 kHz. Change in frequency leads to a change in the sign of the effect. There is a sizeable dielectric relaxation process near T$_N$, which exhibits an activated behavior and strongly non-Nabeya nature at or below T$_N$ while becoming Debye like at higher temperature.

¹The work was supported by the Department of Science and Technology, Government of India.

12:27PM Q10.00007 Flexoelectricity in nanostructures, PRADEEP SHARMA, University of Houston — Crystalline piezoelectric dielectrics electrically polarize upon application of uniform mechanical strain. Inhomogeneous strain, however, locally breaks inversion symmetry and can potentially polarize even non-piezoelectric (centrosymmetric) dielectrics. Flexoelectricity—the coupling of strain gradient to polarization— is expected to show a strong size-dependency due to the scaling of strain gradients with structural feature size. In this study, using a combination of atomistic and theoretical approaches, we elucidate the “effective” size-dependent piezoelectric and elastic behavior of inhomogeneously strained non-piezoelectric and piezoelectric nanostructures. We argue, through computational examples, the tantalizing possibility of creating “apparently piezoelectric” nano-composites without piezoelectric constituents and the emergence of size-dependent “giant piezoelectricity” in paradigmatical nanostructures. Finally, we propose that flexoelectricity is an important and essential contributor to the intrinsic dead-layer effect in high permittivity ferroelectric based nanocapacitors.

1:03PM Q10.00008 Evidence for the Potential Barrier Height Reduction in Metal-Oxide-Metal Tunnel Junctions due to the Interface Dependent Metal-Induced-Gap-States, LEE HOSIK, NEC, HYUNTAE JUNG, YONGMIN KIM, KYOOHO JUNG, HYUNSIK IM, Dongguk University, YURI PASHKIN, O. ASTAFIEV, J. S. TSAI, NEC Nano Electronics Research Laboratories and RIKEN Advanced Science Institute, YOSHIYUKI MIYAMOTO, NEC, NEC TEAM, DONGGUK UNIVERSITY TEAM, NEC NANO ELECTRONICS RESEARCH LABORATORIES and RIKEN ADVANCED SCIENCE INSTITUTE TEAM — We have performed transport measurements on AI and Nb based metal-oxide-metal tunnel junctions with an AlO$_x$ tunnel barrier and found a strong dependence of the effective potential barrier height on the oxide-metal interface properties. Our estimations of the barrier height based on a phenomenological Simmons’ model are consistent with the values obtained from the first-principle calculations. The calculations clearly show that the barrier height is strongly affected by the formation of metal induced gap states originating from the hybridization between metallic bands and AlO$_x$ conduction band. These findings are important for nanoelectronic devices containing tunnel junctions with a thin insulating layer.

1:15PM Q10.00009 Role of defects in the interfacial conductivity at interfaces in Pt/ SrTiO$_3$/Pt heterostructures, NAGA PHANI AETUKURI, Stanford University/IBM Almaden Research, GUENOLE JAN, IBM Almaden Research/Magic; MAHESH SAMANT, KEVIN ROCHE, STUART PARKIN, IBM Almaden Research — Oxides exhibit a wide variety of diverse phenomena including ferromagnetism, anti-ferromagnetism, ferroelectricity, superconductivity and multiferroicity. Furthermore, they display complex phase diagrams which result from the sensitivity of their properties to subtle changes in structure, doping, temperature and pressure. We will present the effect of interfaces and interface defects on the electrical switching properties of metal-insulator-metal (MIM) structures where the insulator is strontium titanate (STO) grown by pulsed laser deposition. The role of growth temperature and pressure and the effect of intentionally created oxygen vacancies on MIM device characteristics will be discussed. An attempt will be made to rationalize the role of intrinsic mechanisms and interface effects on the variability seen in device properties.
1:27PM Q10.00010 High-quality SrTiO$_3$ films using a hybrid MBE approach, BHRAT JALAN, ROMAN ENGEL-HERBERT, NICK WRIGHT, SUSANNE STEMMER, University of California Santa Barbara — A novel hybrid molecular beam epitaxy (MBE) approach for atomic-layer controlled growth of high-quality, epitaxial, stoichiometric SrTiO$_3$ films is presented. A solid source is used for Sr, an rf oxygen plasma source for oxygen and a metal-organic source for Ti. High-resolution x-ray diffraction revealed high quality single crystalline films with rocking curve full width half maxima similar to those of the substrates (i.e., 0.0095° for a LSAT substrate). RHEED showed persistent layer-by-layer growth (> 180 oscillations), which has previously been observed only in a very few other systems (Si and GaAs). Surface reconstructions were observed during growth and related to the growth modes. Depending on growth conditions, step flow growth was also observed. The film surface RMS roughness was less than 0.2 nm. Excellent film stoichiometry was confirmed by homoepitaxy (prefect overlap of film and substrate reflections). Films were very insulating, consistent with oxygen stoichiometry. Oxygen gettering Ti contacts and vacuum anneals were used to produce n-type, oxygen deficient films to study carrier mobilities. We demonstrate the relative influence of hydrogen and oxygen vacancies on the electrical conductivity of SrTiO$_3$.

1:39PM Q10.00011 Conductance bistability in metal oxide junctions, ZHONGKUI TAN, VIJAY PATEL, ESTEBAN MONGE, SHIH-HENG CHANG, SHAW POTTORF, JAMES LUKENS, KONSTANTIN LIKHAREV, Department of Physics and Astronomy, Stony Brook University — We are exploring conductance bistability (memory) effects in junctions based on metal oxides, in the context of their possible applications in hybrid CMOS/nanoelectronic (e.g., CMOL [1]) circuits. So far, we have investigated Cu$_2$O, NbO$_x$ and TiO$_x$ formed by thermal and plasma oxidation, with or without rapid thermal post-annealing (at 200 to 800°C for 30 to 300 seconds). Conductance switching effects have been observed for all these materials. Particularly high endurance (over 1000 switching cycles) has been obtained for TiO$_x$ junctions plasma oxidized in 15mTorr oxygen and then post-annealed at 700°C. However, the ON/OFF conductance ratio for these junctions is only about 5, and the sample-to-sample reproducibility is much lower than required for integrated circuit applications. Our plans are to extend our studies to a-Si junctions with one Ag electrode, and multilayer TiO$_x$ junctions, with the main goal to improve device reproducibility. The work is supported in part by AFSOR.


1:51PM Q10.00012 Electrical characterization of epitaxial MgO/SiC capacitor structures, AGHAM POSADAS, FRED WALKER, CHARLES AHN, Yale University, TREVOR GOODRICH, ZHUHUA CAI, KATE ZIEMER, Northeastern University — Epitaxial heterostructures of MgO (111) have been grown on hydrogen-cleaned 6H-SiC (0001) substrates and characterized using capacitance vs. voltage (C-V) and current vs. voltage (I-V) measurements. Low frequency capacitance measurements of MgO/SiC under strong accumulation conditions as a function of MgO layer thickness show that the exciton MgO has a dielectric constant of 10. The C-V measurements show modulation of the SiC from accumulation to depletion, consistent with the wafer conductivity type. The density of interface states was determined from ac conductance vs. frequency measurements, indicating a density of 6 x 10^{11} eV^{-1} cm^{-2} at an energy level close to the conduction band edge, similar to what has been reported for native SiO$_2$ capacitor structures. In order to determine the dielectric breakdown field of the epitaxial MgO, leakage current as a function of gate voltage was measured for the capacitor structures. The median gate voltage at which the MgO breaks down was found to correspond to an electric field of 12 MV/cm, similar to that of bulk, single crystal MgO. These results show that epitaxial MgO has potential for use as a gate dielectric in Si MOSFET applications.

2:03PM Q10.00013 Observation and coupling of domains in a spin spiral multiferroic, DENNIS MEIER, MICHAEL MARINGER, THOMAS LOTTERMOSER, MANFRED FIEBIG, HISKP, University Bonn, PETRA BECKER, LADISLAV BOHATY, Institute for Crystallography, University of Cologne — The intrinsically strong cross coupling between magnetism and ferroelectricity in spin spiral multiferroics suggests these systems as prime candidates for novel multifunctional devices. Comprehension and controlling of the correlated antiferromagnetic (AFM) and ferroelectric (FE) domain structures by external fields is an indispensable prerequisite for future device design. However, very few is known about the domain topology and switching of AFM spin spirals and the magnetically induced FE domains. Here we present the spatial distribution of AFM and FE domains in MnW$_x$O, revealed by optical second harmonic generation. Electric fields are used to uniquely control the magnetic domain structure, while applied magnetic fields influence the polar behavior of the FE domains.

This work is supported by the DFG through SFB 608.


11:15AM Q11.00001 Dielectric Optical Antenna Emitters and Metamaterials, JON SCHULLER, Stanford University — Optical antennas are critical components in nanophotonics research due to their unparalleled ability to concentrate electromagnetic energy into nanoscale volumes. Researchers typically construct such antennas from wavelength-size metallic structures. However, recent research has begun to exploit the scattering resonances of high-permittivity materials to realize all-dielectric optical antennas, emitters, and metamaterials. In this talk, we experimentally and theoretically characterize the resonant modes of subwavelength rod-shaped dielectric particles and demonstrate their use in negative index metamaterials and novel infrared light emitters. At mid-infrared frequencies, Silicon Carbide (SiC) is an ideal system for studying the behavior of dielectric optical antennas. At frequencies below the TO phonon resonance, SiC behaves like a dielectric with very large refractive index. Using infrared spectroscopy and analytical Mie calculations we show that individual rod-shaped SiC particles exhibit a multitude of resonant modes. Detailed investigations of these SiC optical antennas reveal a wealth of new physics and applications. We discuss the distinct electromagnetic field profile for each mode, and demonstrate that two of the dielectric-type Mie resonances can be combined in a particle array to form a negative index metamaterial [1]. We further show that these particles can serve as “broadcasting” antennas. Using a custom-built thermal emission microscope we collect emissivity spectra from single SiC particles at elevated temperatures, highlighting their use as subwavelength resonant light emitters. Finally, we derive and verify a variety of general analytical results applicable to all cylindrical dielectric antennas and discuss extensions of the demonstrated concepts to different materials systems and frequency regimes. [1] J.A. Schuller, et al., Phys. Rev. Lett. 99, 107401 (2007)

11:51AM Q11.00002 Quantum Confined Stark Effect for Exciton-Plasmons in Carbon Nanotubes, IGOR BONDAREV, JUSTICE MCCONNELL, NC Central University — We study theoretically the perpendicular electrostatic field effect (the quantum confined Stark effect) for excitons and interband plasmons in small-diameter (<~1nm) semiconducting carbon nanotubes (CNTs). The exciton creation energy and the plasmon energy both shift to the red due to the decrease in the CN band gap as the fields increases. However, the exciton red shift is much less than the plasmon one due to the decrease in the absolute value of the (negative) exciton binding energy [1]. This brings the exciton in resonance with the interband surface plasmon. The exciton total energy may be tuned to the nearest interband plasmon resonance this way, to form the strongly coupled exciton-surface-plasmon excitation[2,3]. We propose this effect for the development of CN based tunable optoelectronic device applications in areas such as nanophotonics, nanoplasmonics, and cavity quantum electrodynamics.


3Supported by NSF (grants ECS-0631347 and HRD-0833184).
12:03PM Q11.00003 Resonant Plasmonic and Vibrational Coupling in a Tailored Nanoantenna for Infrared Detection, JAVIER AIZPURUA, AITZOL GARCIA-ETXARRI, CSIC-UPV/EHU and DIPC, San Sebastian, Spain, THOMAS W. CORNELIUS, SHAFKAT KARIM, Gesellschaft für Schwerionenforschung, Darmstadt, Germany, FRANK NEUBRECHT, ANNEMARIE PIUCCI, Univ. of Heidelberg, Germany — Gold nanowires are introduced as plasmonic infrared antennas for effective molecular spectroscopy. A novel resonant mechanism involving the interference of the broadband plasmon with the narrowband vibration from molecules is presented in the context of Surface-Enhanced Infrared Absorption (SEIRA). With the use of this concept, we demonstrate experimentally the enormous enhancement of the vibrational signals from less than one attomol of molecules on individual gold nanowires, tailored to act as plasmonic nanoantennas in the infrared. By detuning the resonance via a change in the antenna length, a Fano-like behavior of the spectral signal is observed, which is clearly supported by full electrodynamical calculations. This resonant mechanism can be a new paradigm for sensitive infrared identification of molecular groups.


12:15PM Q11.00004 A novel near field transducer for efficient energy transfer, WILLIAM CHALLENER, AMIT ITAGI, CHUBING PENG, NILS GOKEMEIJER, GNAPING JU, MICHAEL SEIGLER, EDWARD GAGE, Seagate Technology — Interest in the localized surface plasmon resonance (LSPR) of metallic nanoparticles has been piqued by single molecule detection in surface enhanced Raman spectroscopy, scanning optical microscopy with sub-20 nm resolution, particle capture using the optical tweezers effect, and proposed applications in nanolithography and data storage. We have designed a gold near field transducer (NFT) that combines the LSPR effect, the lightning rod effect, and the dual dipole effect. Optical energy that is focused onto the NFT is coupled into a metallic thin film within a spot that is an order of magnitude smaller than the free space wavelength with an efficiency of about 5%. With approximately 40 mW of optical power from a laser diode at a wavelength of 830 nm, data has been recorded at a track width less than 50 nm onto a high coercivity magnetic medium by heating it to its Curie point of 650 K while the medium was rotating at 2700 RPM and the NFT was separated from the medium surface by 15 nm.

12:27PM Q11.00005 Near-field imaging and probe-assisted nano-mechanical control of plasmonic antennas, AITZOL GARCIA-ETXARRI, CSIC-UPV/EHU and DIPC, San Sebastian, Spain, ISABEL ROMERO, DIPC, San Sebastian, Spain, F. JAVIER GARCIA DE ABAJO, Institute of Optics, Madrid, Spain, RAINER HILLENBRAND, CIC nanoGUNE, San Sebastian, Spain, JAVIER AIZPURUA, CSIC-UPV/EHU and DIPC, San Sebastian — Imaging plasmon-resonant gold nanodisks acting as optical nanoantennas by scattering-type near-field optical microscopy (s-SNOM), we identify weak and strong coupling regimes between the near-field probe and the plasmonic nanoantenna sample. By means of rigorous electrodynamical calculations based on a model system, we find that in the weak coupling regime, s-SNOM can be applied for direct mapping of plasmonic nanoantenna modes, while in the strong coupling regime, the near-field probe allows for high-precision opto-mechanical control of the antenna response.

12:39PM Q11.00006 Direct Near-field Imaging of UV Surface Plasmon of a Bowtie Optical Nano-antenna, LIANGCHENG ZHOU, Department of Physics, Lehigh University, QIAOQIANG GAN, Department of Electrical and Computer Engineering, Lehigh University, VOLKMAR DIEROLF, Department of Physics, Lehigh University, FILBERT BARTOLI, Department of Electrical and Computer Engineering, Lehigh University, QIAO QIU and HUO WEI, Liquid Crystal Institute, Kent State University — We numerically study the optical properties of metal-dielectric-metal nanoantennas. The nanoantennas consist of two metal nanocylinders stacked vertically with a dielectric disk spacer. The numerical analysis using finite difference time domain method (FDTD) shows that nanoantennas exhibit two types of resonances when the gap between the metal cylinders is below 5nm. One of the resonance corresponds to the antenna resonance, generates a peak in scattering spectra and the other corresponds to cavity resonance, produces multiple dips in the scattering spectra. The multiple dips are corresponding to the different cavity resonant modes; the resonant frequencies of these modes depend upon the gap size between the cylinders. It is found that as the gap size decreases, enormous electric field enhancement can be generated inside the cavity. For a particular gap size, electric field enhancement can be maximized by varying diameter of the dielectric disk and optimum condition is obtained when dielectric disk diameter is roughly half that of the metal cylinders. The cavity resonance can be explained as interference of gap surface plasmons between two metal cylinders.

1:03PM Q11.00008 Plasmonic hysteresis: temperature dependent resonance of vanadium-dioxide coated gold nanoparticle arrays, DAVON FERRARA, JOYEETA NAG, EUGENE DONEV, JAE SUH, RICHARD HAGLUND, Vanderbilt University — The optical properties of metal nanostructures are dominated by the free-electron, or plasmonic, response of the material. In the case of metal nanoparticles, this leads to a resonant extinction with wavelength determined by the particles’ size, shape, material, and surrounding dielectric. Vanadium-dioxide has a hysteretic transition from a semiconductor to a metal about 68℃ accompanied by a change in its structural, electrical and optical properties.

1:15PM Q11.00009 Surface plasmon lifetime in metal nanoshells, A.S. KIRAKOSYAN, T.V. SHAHBAZYAN, V.V. BERZ, A.S. KIRAKOSYAN, T.V. SHAHBAZYAN, R/v, where R is...
1:27PM Q11.00010 Finite Size Effects on the Electromagnetic Field Enhancement from Low-dimensional Silver Nanoshell Dimer Arrays1, YOULIN SONG, Zhengzhou University, KE ZHAO, University of Tennessee, YU JIA, XING HU, Zhengzhou University, ZHENGYU ZHANG, Oak Ridge National Laboratory — Finite size effects on the optical properties of one-dimensional (1D) and 2D nanoshell dimer arrays are investigated using generalized Mie theory and coupled dipole approximation within the context of surface-enhanced Raman spectroscopy (SERS). It is shown that the huge enhancement in the electromagnetic (EM) field at the center of a given dimer oscillates with the length of the 1D array. For an array of fixed length, the EM enhancement also oscillates along the array, but with a different period. Both types of oscillations can be attributed to the interference of the dynamic dipole fields from different dimers in the array. When generalized to 2D arrays, EM enhancement higher than that of the 1D arrays can be gained with a constant magnitude, a salient feature advantageous to experimental realization of single-molecule SERS. [K. Zhao et al, J. Chem. Phys. 125, 081102 (2005); Y. L. Song et al, accepted by J. Chem. Phys.]

Work supported by DMSE/BES of DOE and NSF

1:39PM Q11.00011 System-bath approach to electronic effect in Surface Enhanced Raman Scattering1, SEMION SAIKIN, ROBERTO OLIVARES-AMAYA, CESAR RODRIGUEZ-ROSARIO, Department of Chemistry and Chemical Biology, Harvard University, MICHAEL STOPA, Center for Nanoscale Systems, Harvard University, ALAN ASPURU-GUZIK, Department of Chemistry and Chemical Biology, Harvard University, SEC TEAM — Raman scattering from molecules is greatly enhanced in proximity of a metal nanoparticle or a rough metal surface. The strong interest in this effect is driven by applications to selective detection of toxic chemicals, warfare agents, etc. The scattering enhancement has two distinct contributions. The electromagnetic effect originates in the field concentration by surface plasmons excited in the metal. The second, electronic or chemical contribution, which is important for molecules in direct contact with the surface, is more controversial. It is controlled by the charge transfer between a molecule and a metal with nanoscale roughness. We develop an open quantum system approach to the formation of charge transferred states and apply it to describe electronic effect in SERS using specific examples of organic molecules adsorbed on a surface of a silver nanoparticle.

The work was supported by DARPA MTO grant FA9550-08-1-0285

1:51PM Q11.00012 Single molecule surface-enhanced Raman spectroscopy in nanogap structures , DANIEL WARD, NAOMI HALAS, DOUGLAS NATELSON, Rice University — Single molecule sensitivity in surface enhanced Raman scattering (SERS) is of significant interest to multiple fields of study but has been difficult to demonstrate conclusively. We have developed a planar nanogap structure with single molecule Raman sensitivity (Nano Lett. 7, 2007; Nano Lett. 8, 2008). Nanogap devices offer a reliable way to probe SERS phenomena often thought to be the hallmarks of single molecule sensitivity: intensity fluctuations and spectral diffusion. We present a series of experiments on intensity fluctuation and spectral diffusion rates as a function of temperature to better understand the mechanism driving these phenomena. We also explore how the gap width affects overall Raman intensity. Additionally, time permitting, we present results on plasmonic light emission from nanogap devices when excited by hot electrons. The spectrum shows intensity peaks at energies well above the excitation energy revealing a wealth of interesting physics.

2:03PM Q11.00013 Plasmonic Nanolens Arrays for Enhanced Raman Spectroscopy1, E.V. PONI-ZOVSKAYA, I. NAUMOV, Z. LI, JING TANG, A.M. BRATKOVSKY, Hewlett-Packard Labs, Palo Alto — Surface-enhanced Raman scattering (SERS) is the 4th-order process with regards to a local electric field, -|E|^4, and therefore, may be extraordinarily enhanced well in excess of 10-11 orders of magnitude. The 'chemical' enhancement factor of less clear origin may also reach few orders of magnitude. We are looking at engineering various nanoparticle arrays that may focus local field and may be fabricated in top-down manner or self-assembled. Nanocrystals of Au and Ag with different shapes, such as octahedra, cubes, stars etc and their 2-dimensional and 3-dimensional assembly have been studied for plasmonic applications. One promising way of reaching the enhancement ≥ 10^{12}/is to use arrays of plasmonic nanolenses with with binary or even ternary nanoparticles arrangements with certain patterns. The nanoparticles arrangements were modeled numerically using Finite Difference Time Domain method and results are compared with the data collected by our team on some fabricated high-performance SERS substrates.

In collaboration with Peidong Yang’s Group at UC Berkeley.

Wednesday, March 18, 2009 11:15AM - 2:15PM –
Session Q12 DMP DCMP: Structure, Dynamics, and Diffusion at Surfaces 308

11:15AM Q12.00001 Water Adsorption on Wurtzite GaN Surfaces , XIAO SHEN, PHILIP B. ALLEN, Stony Brook University, MARK S. HYBERTSEN, JAMES T. MUCKERMAN, Brookhaven National Laboratory — A solid solution of wurtzite GaN/ZnO absorbs light in the visible and can photosplit water|1| |1| |1| |1|. The water is oxidized by the photo-holes at the surface of the semiconductor alloy. However, microscopic details of the oxidation process are unknown. We present a first-principles study of water adsorption on wurtzite GaN. We study the structures and energetics of water adsorption, calculate the energy barrier for water dissociation, analyze the water-water interactions, and study the electronic structure. The results are compared with water adsorption on ZnO surface. We also study the behavior of the holes near the water-semiconductor interface.


11:27AM Q12.00002 Does Water Adsorb Molecularly or Dissociatively on a Plutonium Surface?1, ASOK RAY, RAYMOND ATTA-FYNN, Department of Physics, University of Texas at Arlington — DFT-GGA has been used to study adsorption of water in molecular and dissociative configurations on δ-Pu (111) surface. In molecular state, water is physisorbed in an almost flat-lying orientation at a one-fold coordinated on-top site. The interaction of the water δσ orbital and the Pu-6δl orbital provides the stability of water on the surface, implying that the Pu-5f electrons remain chemically inert. The coadsorption cases of partially dissociated and fully dissociated products at the three-fold hollow sites yield chemisorption, coupled with rumpling of the surface layer and delocalization of the Pu-5f electrons and formation of strong ionic bonds.

This work is supported by the U. S. Department of Energy and the Welch Foundation
surface\textsuperscript{1}, BERNARD DELLEY, Paul Scherrer Institut, ALFONSO BALDERESCHI, MICHEL POSTERNAK, EPF-Lausanne — Using density functional calculations and a periodical slab model, we investigate water adsorption on edges formed by intersection of two anatase TiO$_2$ (101) surfaces. We find that after adsorption of a water molecule on a low-coordinated Ti atom on the ridge, decomposition may happen over a moderately high barrier. In this process, a proton gets abstracted by bonding to a low-coordinated ridge oxygen atom. The hydroxyl anion remains bonded to the acidic Ti site on the edge. The methods used to find the saddle points and to map out the reaction paths are briefly discussed. We also give a discussion of the reaction rates that may be expected based on these calculations. The presence of hydroxyl groups and protons is favoring nucleation of Ca phosphate bonding by allowing exchange of the adsorbed proton against Ca$^{2+}$ ions. Such processes are thought to be essential for the biocompatibility of titanium and its use in dental and orthopedic applications.

\textsuperscript{1}This work is supported by ITI Foundation for the promotion of Implantology, Switzerland.

11:51AM Q12.00004 First Principles Study of Bulk and Surface Ordering Phenomena in Pt-X Binary Alloys in the Presence of Oxygen. WEI CHEN, CHRIS WOLVERTON, Northwestern University, Department of Materials Science and Engineering, WILLIAM SCHNEIDER, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Department of Chemistry and Biochemistry — Alloying in metal catalyst particles (such as platinum) may change surface structure due to segregation and ordering, which may in turn significantly impact catalytic activity. Using first principles density functional theory (DFT) calculations in conjunction with a cluster expansion (CE) technique, we have studied the ordering/phase-separation phenomena of bulk and surface Pt-X binary alloys, with a specific focus on Pt-Au. The surface DFT+CE calculations are performed both in the presence and absence of oxygen. For Pt-Au, the calculated results reveal a phase separating tendency in bulk Pt-Au and a small coherency energy between these two elements. The Pt-Au phase diagram calculated by combining DFT+CE with Monte Carlo simulation shows a slightly asymmetric miscibility gap in good agreement with experimental results. In contrast to the bulk tendency, the surface does not show a pronounced phase-separation tendency, with several low-energy "striped" ordered structures (with a very small, negative formation energy). The presence of oxygen qualitatively changes the surface segregation tendency of Au, and our DFT+CE results show that the equilibrium structure of the Pt-Au (111) surface varies with oxygen coverage.

12:03PM Q12.00005 A first-principles study of the electropotential dependent shape stability of metal nanoparticles. NICEPHORE BONNET, MIT, ISMAILA DABO, CERMECS ENPC, NICOLA MARZARI, MIT — Understanding the catalytic activity of transition metal nanoparticles is a central issue in the development of novel fuel cell materials. Observed trends are often interpreted in terms of the size dependent shape of nanoparticles, in particular the relative density of low coordination sites. However, no consensus exists regarding the direction or even the existence of such an effect. In this context, ab-initio methods can be useful to extract relevant parameters. Here, we calculate surface energies under realistic electrochemical conditions and use the Wulff construction to infer stable nanoparticle contours. The electropotential is adjusted through its conjugate variable, the charge, and density countercharge periodic-image corrections are applied. The surrounding solvent is treated as a combination of a continuum dielectric and a classical ionic distribution at equilibrium.

12:15PM Q12.00006 Lattice Dynamics of Cu$_2$O: Bulk and (110) Surface. KLAUS-PETER BOHNEN, ROLF HEID, Forschungszentrum Karlsruhe, IFP, ALOYSIUS SOON, CATHERINE STAMPFL, School of Physics, University of Sydney — A number of theoretical studies have been carried out in the past to investigate the stability of various surface oxides for the O/Cu system however despite the fact that catalytic processes usually proceed at elevated temperatures stability at finite temperatures has never been studied for these systems. Modern ab-initio methods however allow for the determination of the lattice dynamics and the phononic contribution to the free energy. Using density functional perturbation theory we have studied the lattice dynamics of Cu$_2$O-bulk as well as Cu$_2$O(110). In calculating the free energy as function of lattice constant we obtained for the bulk a negative thermal expansion up to roughly 300 K in excellent agreement with experiments. This is due to anomalous mode Gr"uneisen parameters for vibrational modes in the low energy regime. Due to the anomalous behavior of the mode Gruneisen parameter the bulk system is highly unstable against variations of the lattice constant by more than 2%. To investigate the stability of the O/Cu surfaces we have investigated the lattice dynamics of Cu$_2$O(110) as a prototype. Despite a large number of low lying modes no instability has been found. These calculations allow also for the O/Cu system for the first time a realistic estimation of the surface-free energy which is important for the determination of surface thermodynamic properties.

12:27PM Q12.00007 Ab-initio Study of the Erlich-Schoewebel Barriers for fcc(100). TALAT S. RAHMAN, HANDAN YILDIRIM, University of Central Florida — We present the results of density functional theory based calculations for the activation energies for the diffusion of adatoms (Cu or Ag) on Cu(100) and Ag(100) surfaces with and without steps. For Ag adatom diffusion via hopping on Cu(100), we find the energy barrier to be 0.37 eV, which is less than that (0.60 eV) of Cu adatom diffusion on Ag(100). In the presence of a step edge, we find the Erlich-Schoewebel (ES) barriers (via hopping process) for both Ag and Cu atoms on Cu(100) to be 170 meV. For Ag and Cu adatoms on Ag(100), the corresponding barriers are 50 meV and 60 meV, respectively. The ES barrier (via exchange process) for Ag on Ag(100) is found to be 20 meV and for Cu on Cu(100) it is 60 meV. The barriers for diffusion along the step edges at the lower terraces are 0.36 eV and 0.20 eV for Cu on Ag(100) and Ag on Cu(100), respectively. We trace the differences in the diffusion barriers of the homo-and hetero-epitaxial systems to the differences in the corrugation of the potential energy surface, and discuss the implications for homo- and heteroepitaxial growth on these surfaces.

1Work is supported in part by NSF-ITR 0428826

12:39PM Q12.00008 On the Si(111) 5×2-Au surface, Si adatom diffusion is defect-mediated. EZRA BUSSMANN, Sandia Natl Labs, NM, S. Bockenhauer, F.J. Himpsele, U.W. - Madison, B.S. Swartzentruber, Sandia Natl Labs, NM — The Si(111) 5×2-Au surface is a member of a family of metal-induced chain reconstructions of Si. Studies of these reconstructions have led to a new understanding of the physics of one-dimensional electronic states. The 5×2 surface is speckled with Si adatoms, which are intimately linked with the surface electronic properties. At temperatures > 423 K, the adatoms diffuse along the chains between adjacent 5×2 cells. We have measured scanning tunneling microscopy movies of the diffusing adatoms. Distinctive diffusion statistics, e. g. correlations between displacements, imply that the displacements are triggered by an interaction with a defect. By a statistical characterization of the diffusion, we show that the adatoms move by a defect-mediated mechanism similar to the vacancy-mediated diffusion observed on some metal surfaces. We use a Monte Carlo simulation to model the diffusion process, accurately reproducing the unique diffusion statistics over the temperature range (145 – 215°C) of our experiments. We have also determined the diffusion activation barrier =1.24 ± 0.08 eV. Sandia National Labs is operated by Sandia Corp, a Lockheed-Martin Company, for the DOE under Contract No. DE-AC04-94AL85000. F.JH and SB acknowledge NSF support under DMR-070145.
12:51PM Q12.00009 The diffusion pathways of phosphorus atoms in the silicon (001) surface  
JENNIFER BENNETT, OLIVER WARSCHKOW, Centre for Quantum Computer Technology, School of Physics, The University of Sydney, NIGEL MARKS, Nanochemistry Research Institute, Curtin University of Technology, DAVID MCKENZIE, Centre for Quantum Computer Technology, School of Physics, The University of Sydney — Effective use of surface chemical reactions to control the placement of dopants in semiconductors requires a detailed understanding of the reaction pathways involved. The most highly developed approach to accurate placement of phosphorus in silicon involves reacting phosphine gas with selected areas of the silicon (001) surface, incorporating the phosphorus atom into the surface and silicon overgrowth. In this computational study we investigate the least understood chemical reactions involved in this process, namely the phosphorus incorporation and associated diffusion reactions. We use density functional theory, combined with an efficient method for locating transition states, to identify the reaction pathways involved in three processes: (1) the diffusion of a phosphorus adatom along the silicon (001) surface, (2) the incorporation of a phosphorus atom into the surface, and (3) the migration of the incorporated phosphorus atom within the surface. The calculated pathways and corresponding reaction barriers provide insight into the conditions required for accurate incorporation and encapsulation of phosphorus atoms into the silicon surface.

1:03PM Q12.00010 Kinetic Monte Carlo studies of the behavior of CO on sulfur-covered Pd(100) surface  
DOMINIC ALFONSO, National Energy Technology Laboratory — Investigations of the behavior of CO on the surface of Pd modified with sulfur were carried out using first-principles Kinetic Monte Carlo method. In particular, the influence of adsorbed sulfur on the adsorption, diffusion and desorption of CO on the Pd(100) surface was studied. A kinetic Monte Carlo code was developed which enables the simulation of hosts of competing elementary steps with lateral interaction between the adspecies taken into account. The barriers and energetics of the relevant reaction pathways were determined by density-functional theory. The rates entering the simulation were derived using transition state theory. The adsorbates were assumed to interact via pairwise additive interactions. We demonstrate that adsorbed sulfur has an adverse effect on the behavior of CO on Pd(100).

1:15PM Q12.00011 Charge-State Dependent Hydrogen Diffusion on Silicon (001)  
OLIVER WARSCHKOW, University of Sydney — The diffusion of hydrogen atoms is relevant to a number of chemical and technological processes of the silicon (001) surface. These include the dissociative adsorption of molecules, the growth of overlayers by chemical vapor deposition (CVD), and the directed atomic-scale functionalization of the surface by scanning tunnelling microscopy (STM) lithography. The basic inter- and intradimer shift reactions of hydrogen are well studied, and activation energies of respectively 1.7 eV and between 1.0 and 1.4 eV are commonly cited. In this presentation, I will pose and discuss two questions: (1) Are single energy barriers adequate to describe H-shift reactions on silicon, and (2) are STM measurements of H-diffusion truly representative for hydrogen desorption in the absence an STM tip? These questions warrant examination because hydrogen adatoms on Si(001) are known to adopt a variety of charge states depending on factors such as the doping level of the silicon substrate, the defect density on the surface, or the presence of an STM tip. High-level density functional calculations are reported to shed some clarity on these questions.

1:27PM Q12.00012 Unidirectional Linear Diffusion on an Isotropic Cu(111) Surface in a Periodic and Asymmetric Potential  
DEZHENG SUN, Department of Physics, UC, Riverside, KI-YOUNG KWON, KIN L. WONG, GREG PAWIN, ERIC CHU, ZHIHAI CHENG, DAE-HO KIM, MIAOMIAO LIO, Department of Chemistry, UC, Riverside, SAMYPO HONG, TALAT S. RAHMAN, Department of Physics, University of Central Florida, Orlando, MICHAEL MARSELLA, LUDWIG BARTELS, Department of Chemistry, UC, Riverside — We performed an STM study of the diffusion of 1.4 benzenedithiol, 9-thioantracone, 9,10-dithioantracone (DTA) and 2,3-dimethyl-9,10-dithioacetylanthracene (DMDTA) as well as naphthaquinone, antraquinone and pentacenetetracene on Cu(111). Inherently uniaxial motion of all species with two thiol groups and at least three aromatic rings are observed. Sequential placement of the substrate linkers prevents DTA and DMDTA from rotating or veering off course. Asymmetric metahylylation impacts DTA’s diffusive behavior by about 100-fold decrease in surface mobility causes by about 2-fold increase of the diffusion barrier, with the overall symmetry of DTA diffusion not affected: A forward/backward ratio of 1.009±0.001, were found i.e. less than 1% deviation from unity. This is in stark contrast to the classical behavior but in perfect agreement with Tolman’s ‘Principle of Microscopic Reversibility’.

1:39PM Q12.00013 Surface Morphological Response of Stressed Elastic Solids under Electromigration Conditions  
VIVEK TOMAR, RAUF GUNGOR, DIMMITROS MAROUDAS, University of Massachusetts, Amherst — We present a theoretical analysis of the surface morphological response of electrically conducting, stressed elastic crystalline solids under the simultaneous action of an electric field that drives surface electromigration. The analysis is based on a fully nonlinear model of driven surface morphological evolution and combines linear stability theory with self-consistent dynamical numerical simulations. We report results of the surface morphological response of a uniaxially stressed solid as a function of electric field strength, surface crystallographic orientation, and temperature. We find that a properly directed and sufficiently strong electric field can stabilize the surface morphology of the stressed solid against crack-like surface instabilities, as well as surface rippling instabilities, and determine the required critical electric-field strength over a broad temperature range and for various surface crystallographic orientations. We also demonstrate the superior morphological response of <111>-oriented surfaces of face-centered cubic metals.

1:51PM Q12.00014 Theory of the lifetime of adsorbate vibrations on semiconductor surfaces  
PETER KRATZER, SUNG SAKONG, University Duisburg-Essen — On semiconductor surfaces, the vibrational lifetime of covalently bonded adsorbates is rather long (nanoseconds or more) since the band gap precludes electronic dissipation. Due to the quantum nature of vibrational states, such slow relaxation is expected, as the large quantum of the bond stretching must be converted into several smaller (phononic or vibronic) quanta by a high-order process. We use density functional theory calculations to map out the high-dimensional potential energy surface governing the anharmonic coupling of the stretching to the local bending and shift modes, while the coupling to the substrate phonons is treated perturbatively. Applying our method to the vibrational lifetime of CO on Si(100), we find that the CO stretching relaxes predominantly via an intermediate state consisting of four shift and/or bending quanta and one phonon. As a second application, we elucidate the role of intermediate vibrational states in the relaxation of the stretching vibration at Ge(100):H surfaces. For Ge surface dimers saturated by one H and one D atom, the lifetime of the Ge–H stretching vibration is up to five times shorter and less temperature-dependent than in Ge dimers homogeneously saturated by H. Our analysis shows that the symmetry breaking associated with the isotope mixture opens up additional relaxation channels.

2:03PM Q12.00015 Modeling H₂-Surface Interactions on Interstellar Dust Grains: A Classical Molecular Dynamics Study  
VIJAY VEERAGHATTAM, STEVEN LEWIS, PHILLIP STANCL, University of Georgia, JUNKO TAKAHASHI, Meiji Gakuin University — A classical Molecular Dynamics (MD) method is employed to model hydrogen molecules interacting with the surface of amorphous ice and to calculate the sticking coefficient as a function of various system parameters. This study, combining molecular physics and surface science, is part of a larger program of research to provide theoretical input for models of dust-grain-mediated physico-chemical processes in the interstellar medium. Many dust-grain systems are thought to be doped with amorphous ice, which motivates the choice of substrate for this study. Our method simulates the various dynamical processes associated with H₂-ice scattering events, including collision, sticking, diffusion, and ejection. Variables such as angle of incidence, molecular rotational state, substrate temperature (T_D), and H₂ temperature (T_H₂) are monitored and allowed to vary. In this talk, we will present our results for the H₂-ice sticking coefficient as a function of T_D and T_H₂.
11:15AM Q13.00001 Computation of the Iron and Iron-Nickel Phase Diagrams from Ambient to Earth’s Inner Core . XUAN LUO, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — We have performed first-principles computation for the magnetic iron and iron-nickel over a wide range of pressure (0-400GPa) and temperature (0-6000K), within density-functional theory (DFT) in the generalized-gradient approximation using the projector augmented wave (PAW) method with the ABINIT code. We computed the free energies of hcp, bcc and fcc phases for iron and nickel including the thermal excitation of electrons and quasiharmonic phonons computed using the supercell method. We find that at high temperatures and pressures random stacking of fcc andhcp (rhc) is most stable even though the difference in Gibbs free energy between fcc andhcp Fe is smaller than the thermal energy. We computed the free energy of stacking faults, the rhcp phase and the percentage offcc and partial ordered sequences along the melting curve. For the first time, we used first-principles calculation to be able to produce the pure-Fe phase diagram including the magnetic contributions at low pressures. In the Fe-Ni system, we find that FeNi3 is an intermediate phase below 700K at 0 GPa, consistent with experiment, and below 50 GPa at 0K. Finally, we obtained the T-P-x phase diagram for FeNi from 0-400 GPa and 0-6000K.

11:27AM Q13.00002 Plasticity-Mediated Structural Transformation and Diamond-Anvil Cell and Shock Melting1 . CHRISTINE WU, PER SODERLIND, JAMES GLOSLI, JOHN KLEPEIS, Lawrence Livermore National Lab — Determination of the melting curve of a metal under high pressures is essential for establishing its phase diagram, and has wide scientific implications, including our understanding of the Earth’s interior. Currently, melting temperatures at high pressure are primarily measured by in situ laser-heated diamond-anvil cell (DAC) or shock wave experiments. Often, but not always, these two methods yield significantly different results for metals with non close-packed structures, such as bcc metals. For instance, anomalously flat melting slopes were reported for numerous bcc metals by DAC. The flatness of the melting slope is in sharp contrast to the classical Lindemann behavior which shock-melting temperatures follow closely. In this presentation, we will report our finding of a plasticity-mediated structural transition of bcc Ta to a partially disordered glassy structure obtained from molecular dynamics (MD) simulations. This transition is fully consistent with reported DAC low melting, thus provide a highly probable resolution to the long-standing controversy in melting of metals under high pressures.

11:39AM Q13.00003 High Pressure-High Temperature Phase Diagram of Beryllium1,2, M.J. LIPP, B.J. BAER, H. CYNN, Z. JENEI, J.-H. KLEPEIS, W.J. EVANS, LLNL, H.-P. LIERMANN, Y. MENG, S.V. SINOGEIKIN, W. YANG, HPCAT, A. LAZICKI, CIW, Y. OHISHI, SPING-8/JASRI — A detailed understanding of the phase diagram of beryllium and its alloys impacts fundamental science and technological applications. Despite a simple atomic structure, theoretical modeling of the phase diagram of beryllium has been extremely challenging and remains an area of active investigation [Kadas, PRB 07]. Extension of the experimental understanding of beryllium will serve to inform and advance theoretical efforts and technological applications. To address these needs, we have extended our previous work [Evans, PRB 05], and performed x-ray diffraction and melt studies beryllium and beryllium alloys at high pressure. We will describe our measurements of the crystal structure, lattice constants, and melt curve of high-pressure beryllium and beryllium alloys. We will discuss insights into this simple yet challenging system.

11:51AM Q13.00004 High Pressure-Temperature Studies of Vanadium1, Z. JENEI, B.J. BAER, H. CYNN, J.-H. KLEPEIS, M.J. LIPP, W.J. EVANS, LLNL, H.-P. LIERMANN, Y. MENG, S.V. SINOGEIKIN, W. YANG, HPCAT — Vanadium, a seemingly simple metal, has captured the interest of high-pressure scientists following the discovery (Ding et al. PRL 2007) of a subtle pressure-induced phase transition from bcc to a rhombohedral phase. Recent first-principles electronic-structure studies (Lee et al. PRB 2007) are consistent with these experiments and extend beyond the range of the measurements, predicting a reentrant phase transition back to bcc at high pressure. Further experiments in the regime of these predictions can validate and advance the understanding of simple metals at high pressures. We have made x-ray diffraction measurements of the crystal structure and lattice parameters of vanadium at high-pressure and temperature. Detailed comparisons will challenge/validate models and guide development of predictive codes. We will discuss our measurements including high temperature behavior, the EOS, and transitions of vanadium at high pressure.

12:03PM Q13.00005 Coupling of Atomistic and Meso-scale Phase-field Modeling of Rapid Solidification1 . J. BELAK, P.E.A. TURCHI, M.R. DORR, D.F. RICHARDS, J.-L. FATTEBERT, M.E. WICKETT, F.H. STREITZ, Lawrence Livermore National Laboratory — Recently, phase field models have been introduced to model the crystallography during polycrystal microstructure evolution [1,2]. Here, we assess these models with molecular dynamics and phase field simulations that overlap in time and space. Large parallel computers have enabled MD simulations of sufficient scale to observe the formation of realistic microstructure during pressure driven solidification [3]. We compare the two methods by calculating the phase field order parameter (quaternion) from the atomic coordinates and drive the evolution with the MD. Results will be presented for the simulations of sufficient scale to observe the formation of realistic microstructure during pressure driven solidification [3]. We compare the two methods by calculating the phase field order parameter (quaternion) from the atomic coordinates and drive the evolution with the MD. Results will be presented for the simulations of sufficient scale to observe the formation of realistic microstructure during pressure driven solidification [3].

12:15PM Q13.00006 New high-pressure phases of calcium and their finite-temperature phase boundaries1, AMANUEL TEWELDEBERHAN, Dalhousie University, STANIMIR BONEV, Dalhousie University — The phase diagram of Ca has been studied using first-principles density functional theory. The simple cubic structure hitherto believed to exist between 32 and 109 GPa is found to be mechanically and thermodynamically unstable. Instead we propose two new solid phases with orthorhombic $\text{Ca}_2$ and $\text{Ca}_3$ structures and determine their finite-temperature phase boundaries. We also predict liquid transitions in molten Ca under compression, which together with the new solid phases provide a consistent description of the Ca phase diagram. The implications of our findings and extensions of the work to other alkali and alkaline-earth metals will be discussed.

1Work supported by NSERC and ACEnet.
12:27PM Q13.00007 Physical and Chemical Transformations of Sodium Cyanide at High pressures. JING-YIN CHEN, Institute for Shock Physics, Washington State University, Pullman, Washington 99164 - 2816, CHOONG-SHIK YOO, Institute for Shock Physics and Department of Chemistry, Washington State University, Pullman, Washington 99164 - 2816 — Pressure-induced physical and chemical transformations of Sodium Cyanide (NaCN) have been studied up to 50 GPa in diamond-anvil cells, using micro-Raman spectroscopy and angle-resolved synchrotron x-ray diffraction. The present results suggest three phase transitions to occur in this pressure range: from NaCN-I (cubic) to NaCN-II (orthorhombic) at 2 GPa, to NaCN-III (monoclinic) at 8 GPa, and to NaCN-IV (tetragonal) at 15 GPa. At higher pressures, NaCN-IV undergoes irreversible chemical changes, which occurs over a large pressure range between 25 and 34 GPa. The new material exhibits a broad yet strong Raman band at around 1600 cm⁻¹, indicating the formation of C=N bonds in a similar configuration of carbon graphitic.

12:39PM Q13.00008 First-order liquid-liquid phase transition in compressed nitrogen. BRIAN BOATES, STANIMIR BONEV — We present results of first-principles molecular dynamics simulations, which provide evidence for the existence of a first-order liquid-liquid phase transition in compressed nitrogen [1]. The transition is from a molecular to a polymeric liquid. It is characterized by a discontinuous loss of molecular stability followed, upon further compression, by gradual transformation until the local order of the liquid becomes similar to that of cg-N. We have computed the phase boundary of the liquid-liquid transition to be first-order between 2000 and 4000 K and determined that above 4000 K it becomes continuous. Comparison with measurements and suggestions for experimental confirmation of our predictions will be discussed as well. [1] B. Boates and S.A. Bonev, submitted.

1Work supported by NSERC

12:51PM Q13.00009 High-temperature high-pressure properties of silica from Quantum Monte Carlo and Density Functional Perturbation Theory. R.E. COHEN, Geophysical Lab., Carnegie Institution, K. DRIVER, Ohio State University, Z. WU, B. MILITZER, University of California, Berkeley, P.L. RIOS, M. TOWLER, R. NEEDS, University of Cambridge — We have used diffusion quantum Monte Carlo (DMC) with the CASINO code with thermal free energies from phonons computed using density functional perturbation theory (DFPT) with the ABINIT code to obtain phase transition curves and thermal equations of state of silica phases under pressure. We obtain excellent agreement with experiments for the metastable phase transition from quartz to stishovite. The local density approximation (LDA) incorrectly gives stishovite as the ground state. The generalized gradient approximation (GGA) correctly gives quartz as the ground state, but does worse than LDA for the equations of state. DMC, variational quantum Monte Carlo (VMC), and DFT all give good results for the ferroelastic transition of stishovite to the CaCl₂ state. The local density approximation (LDA) incorrectly gives stishovite as the ground state. The generalized gradient approximation (GGA) correctly gives quartz as the ground state, but does worse than LDA for the equations of state. DMC, variational quantum Monte Carlo (VMC), and DFT all give good results for the ferroelastic transition of stishovite to the CaCl₂ state. Zero point and thermal contributions are included by using DFT linear response within the quasiharmonic approximation. Preliminary results indicate the QMC phase relations and bulk moduli are in reasonable agreement with experiment.


Computations were performed at NERSC, OSC, and CCNI. Financial support provided by the DOE (DE-FG02-99ER45795).

1:03PM Q13.00010 Quantum Monte Carlo Equations of State of α- and β-Magnesium Silicate. KEVIN P. DRIVER, JOHN W. WILKINS, The Ohio State University — The 410 km seismic discontinuity in Earth’s mantle is ascribed to the α to β-(Mg,Fe)₂SiO₄ phase transformation. Considering Mg-endmembers, density functional theory (DFT) predictions within LDA and GGA disagree on the phase boundary by 50% [1]. Quantum Monte Carlo (QMC) offers a route to avoid the approximation of the exchange-correlation potential in DFT and provide a benchmark for the phase boundary, elastic moduli, and thermodynamic properties. Zero point and thermal contributions are included by using DFT linear response within the quasiharmonic approximation. Preliminary results indicate the QMC phase relations and bulk moduli are in reasonable agreement with experiment.


1:15PM Q13.00011 High Pressure Studies on Group IV Transition Metals Based Metallic Glasses. ANDREW STEMHSORN, YOGE什 VOHRA, University of Alabama at Birmingham — The compression behavior of Group IV transition metals based metallic glasses Ti37Zr29Cu15Sn14.5B6 and Zr57Cu15.4Ni12.6Al10Nb5 are investigated at room temperature up to 74 GPa in a diamond anvil cell using in-situ energy and angular dispersive x-ray diffraction with a synchrotron radiation source. The x-ray diffraction studies did not reveal any pressure induced crystallization phenomenon in metallic glasses to a volume compression of 35 percent. In Zr-based metallic glass, a nanostructured tetragonal Zr2Ni phase was observed and also found to be stable to the highest pressure. The measured equation of state (Pressure-Volume curve) of Group IV transition metals based metallic glasses is compared to the known high phases of transition metals.

We acknowledge support from the NSF under Grant No. DMR-0703891.

1:27PM Q13.00012 High-pressure-High-temperature phases of Carbon Dioxide. AMARTYA SENGUPTA, Washington State University, Pullman WA 99164, CHOONG-SHIK YOO, Washington State University, Pullman, WA 99164 — The phase diagram of CO₂ has not been understood adequately above 40 GPa and high temperatures, particularly regarding the stabilities and boundaries of various extended phases that include a-carbonia, phase V, and to an extent Phase III. We have studied the phase diagram of CO₂ above 40 GPa and at high temperatures, using both ohmically and laser-heated diamond anvil cells. We found the co-existence of several extended phases over a large pressure region, which we attribute to the metastability of the extended phases and the extraordinarily large pressure gradients at these pressures. We determined the relative stability fields of the co-existing phases, which may offer the physico-chemical mechanism for the existence of carbonate minerals in deep Earth’s mantle.

1:39PM Q13.00013 First-principles study of BC₂N. EUNJA KIM, TAO PANG, Department of Physics and Astronomy, UNLV, NV 89154, USA. WATARU UTSUMI, Sychrotron Radiation Research Center, Japan Atomic Energy Research Institute, Japan, VLADIMIR SOLOZHENKO, LPMTN-CNR, Universite Paris Nord, France, YUSHENG ZHAO, LANL, Los Alamos, New Mexico, 87545, USA — First-principles calculations are performed and analyzed to identify different phases of BC₂N synthesized experimentally. With a proper choice of the supercell, cutoff energy, and sampling k points, the cubic phases are found to be stable theoretically. The bulk moduli from elastic stiffness constants for each of the phases is in excellent agreement with available experimental data. All the phases are defect free and do not possess any B–B or N–N bond. Two high-density phases with nearly degenerate energies are interpreted to represent two experimental systems of different x-ray patterns. The high-density phases are characterized by the existence of C–C bonds whereas the low-density phase is characterized by the absence of C–C bonds. From the calculated equation of state and the available experimental data, we show for the first time that the unique feature of each of the cubic BC₂N phases is a direct result of the corresponding local electronic structure and chemical bonding in the system.

This work is supported in part by the U.S. Department of Energy (DOE) through HiPSEC in UNLV.
1:51PM Q13.00014 Large volume change across OI \rightarrow\text{OII} phase transition in transition-metal dioxides TiO$_2$, ZrO$_2$, and HfO$_2$ as determined by experiment and theory

1:51PM Q13.00014 Large volume change across OI \rightarrow\text{OII} phase transition in transition-metal dioxides TiO$_2$, ZrO$_2$, and HfO$_2$ as determined by experiment and theory

YAHYA AL-KHATATBEH, New Mexico State University, KANANI K.M. LEE, Yale University, BORIS KIEFER, New Mexico State University — The nature of bonding in transition-metal dioxides TiO$_2$, ZrO$_2$, and HfO$_2$ is of interest as they are potential superhard materials with many industrial applications. Using high-resolution synchrotron x-ray powder diffraction for TiO$_2$ and ZrO$_2$, and complementary ab-initio computations of these dioxides, we have determined the equation of state of the orthorhombic I (O1) and orthorhombic II (OII) phases. Our measurements are in agreement with the computationally predicted phase sequence of these oxides. The measured volume change across OI \rightarrow\text{OII} transition is 8.3\% for TiO$_2$ and 10\% for ZrO$_2$ in good agreement with our density-functional theory (DFT) calculations that predict a large volume change for all of these dioxides across the OI \rightarrow\text{OII} phase transition. For TiO$_2$, this volume collapse is significantly higher than previously measured (2.6\%), but consistent with the volume decreases observed in both ZrO$_2$ and HfO$_2$ across this transition. Furthermore, the OII phase was observed to be the most stable phase of TiO$_2$ and ZrO$_2$ at high pressure (56 GPa) after heating to high temperatures (above \sim 1800 K) and no post-OII phase was observed under these conditions.

2:03PM Q13.00015 Crystal Structure and Phase Transition of XeF$_2$ at High Pressures

MINSEOB KIM, Institute for Shock Physics, CHOONG-SHIK YOO, Institute for Shock Physics and Department of Chemistry, STATIC HIGH PRESSURE GROUP IN ISP TEAM — We have investigated the crystal structure and phase transition of solid XeF$_2$ up to 51 GPa in diamond anvil cells by using Raman and synchrotron x-ray diffraction. The x-ray data indicates the tetragonal-to-orthorhombic phase transition at 7 GPa, which accompanies a small distortion (< 1\%) in the ab-plane of the tetragonal structure. The Rietveld refinement further indicates a rapid change of intermolecular F...F contact distance with increasing pressures and, thereby, a rotation of linear symmetric XeF$_2$ molecules along the c-axis and the observed distortion in the ab-plane. This symmetry lowering tetragonal-to-orthorhombic transition also induces the Davydov splitting of symmetric stretching $\nu_1$ and bending $\nu_2$ modes in the Raman spectrum.

Wednesday, March 18, 2009 11:15AM - 1:51PM
Session Q14 DFD: Granular Fluctuations

11:15AM Q14.00001 Cooling and aggregation in wet granulates

ANNETTE ZIPPELIUS, STEPHAN ULRICH, TIMO ASPELMIEIER, University of Goettingen, KLAUS ROELLER, AXEL FINGERLE, STEPHAN HERMINGHAUS, Max-Planck-Institute for Dynamics and Self-Organization — Wet granular materials are characterized by a fixed bond energy in their particle interaction such that breaking a bond implies an irreversible loss of a fixed amount of energy. Associated with the bond energy is a nonequilibrium transition, setting in as the granular temperature falls below the bond energy. The subsequent aggregation of particles into clusters is shown to be a self-similar growth process with a cluster size distribution that obeys scaling. In the early phase of aggregation the clusters are fractals with $D_f = 2$, for later times we observe gelation. We use simple scaling arguments to derive the temperature decay in the early and late stages of cooling and verify our results with event-driven simulations.

11:27AM Q14.00002 Propagating Waves in a Monolayer of Self-Propelling Gas-Fluidized Rods

LYNN J. DANIELS, DOUGLAS J. DURIAN, University of Pennsylvania — We report on the existence of propagating compression waves in a quasi-two-dimensional monolayer of self-propelling rods fluidized by an upflow of air. This behavior is unique to rods; a comparable system of spheres exhibits no waves and displays ‘thermal’ number fluctuations, proportional to $N^{1/2}$. The waves, however, give rise to anomalously large number fluctuations, having both magnitude and exponent greater than ‘thermal’ fluctuations. This occurs as rarefaction zones relax after a compression front has traveled through a region. We characterize the waves by calculating a dynamic structure factor. The position of observed peaks, as a function of frequency $\omega$ and wavevector $k$, yield a linear dispersion relationship in the long-time, long-wavelength limit and a wavespeed $\omega/k = 20$ cm/s. By contrast, spheres exhibit $1/\omega^2$ decay for all wavemodes in the hydrodynamic limit, consistent with the diffusive decay of density fluctuations.

11:39AM Q14.00003 Phase diagram of wet granular matter under vertical vibrations

KAI HUANG, KLAUS ROELLER, STEPHAN HERMINGHAUS, Max Planck Institute for Dynamics and Self-organization — The phase diagram of vertically vibrated wet granular matter is investigated by both experiments and simulations. We find a critical point where the coexistence (C) regime of the fluid (F) and gas (G) phases terminates. The energy driven F-C transition is found to scale with the rupture energy of a liquid bridge if the corresponding vibration amplitude $A$ is less than particle diameter($d$). This is in good agreement with our simulations. Close to the F-G transition line, the variation of the size of the gas bubble grows significantly with vibration amplitude shows a hysteretic behavior. Within the hysteresis loop, we observe temporary gas bubbles with strong fluctuations in size. The F-G transition also induces the Davydov splitting of symmetric stretching $\nu_1$ and bending $\nu_2$ modes in the Raman spectrum.

11:51AM Q14.00004 Stress wave mitigation in granular media

CHIARA DARAILO, CALTECH, F. FERNANDO, University of Salerno, Italy, MASON PORTER, Oxford University, UK — We study stress wave mitigation in one- and two-dimensional granular media employing evolutionary algorithms to investigate the optimal design of composite protectors using granular chains composed of beads of various sizes, masses, and stiffnesses. We define a fitness function using the maximum force transmitted from the protector to a “wall” that represents the body to be protected and accordingly optimize the topology (arrangement), size, and material of the chain. We obtain optimally randomized granular protectors characterized by high-energy equipartition and the transformation of incident waves into interacting solitary pulses. We provide a quantitative characterization of dissipative effects using the propagation of highly nonlinear solitary waves as a diagnostic tool and develop optimization schemes that allow one to compute the relevant exponents and prefactors of the dissipative terms in the equations of motion. We thus propose a quantitatively-accurate extension of the Hertzian model encompassing realistic material dissipative effects. Experiments and computations with steel, brass, and polytetrafluoroethylene reveal a common dissipation exponent (for a discrete Laplacian of the velocities) with a material-dependent prefactor.

2:03PM Q14.00005 Anisotropies in granular temperature in a dense sheared granular flow

CHRIS RYRCROFT, University of California, Berkeley and Lawrence Berkeley Laboratory, ASHISH ORPE, National Chemical Laboratory, India, ARSHAD KUDROLLI, Clark University — We investigate a three-dimensional, slow, gravity-driven, sheared granular flow, making use of both simulation (carried out using the Discrete-Element Method) and experiment (using glass beads, imaged via an index-matched fluid). We begin by performing a quantitative comparison between the two procedures, concentrating on the level of agreement at the microscopic scale. After establishing how well the simulation can reproduce the microscopic fluctuations in particle velocities seen in experiment, we proceed to carry out a tensorial analysis of granular temperature. Our results show different types of behavior near the boundary and in the bulk of a granular flow, due to differences in the particle packing structure, and highlight anisotropies that may have implications for granular continuum modeling.

Support from ARO is greatly acknowledged

3:15PM Q14.00006 Laser-induced light deflection in granular matter

CHIARA DARAILO, CALTECH, F. FERNANDO, University of Salerno, Italy, MASON PORTER, Oxford University, UK — We study light deflection in granular media employing evolutionary algorithms to investigate the optimal design of composite protectors using granular chains composed of beads of various sizes, masses, and stiffnesses. We define a fitness function using the maximum force transmitted from the protector to a “wall” that represents the body to be protected and accordingly optimize the topology (arrangement), size, and material of the chain. We obtain optimally randomized granular protectors characterized by high-energy equipartition and the transformation of incident waves into interacting solitary pulses. We provide a quantitative characterization of dissipative effects using the propagation of highly nonlinear solitary waves as a diagnostic tool and develop optimization schemes that allow one to compute the relevant exponents and prefactors of the dissipative terms in the equations of motion. We thus propose a quantitatively-accurate extension of the Hertzian model encompassing realistic material dissipative effects. Experiments and computations with steel, brass, and polytetrafluoroethylene reveal a common dissipation exponent (for a discrete Laplacian of the velocities) with a material-dependent prefactor.
12:15PM Q14.00006 Correlation Functions of a Homogeneously Driven Granular Fluid in Steady State, KATHARINA VOLLMAYR-LEE, Bucknell University, TIMO ASPELMEIER, ANNETTE ZIPPELIUS, Georg-August-Universitaet Goettingen, Germany — We study a homogeneously driven granular fluid of hard spheres at intermediate volume fractions and focus on time-delayed correlation functions in the stationary state. The results of computer simulations using an event driven algorithm are compared to the predictions of generalized fluctuating hydrodynamics. The incoherent scattering function \( F_{\text{incoh}}(q, t) \) follows time-superposition and is well approximated by a Gaussian \( F_{\text{incoh}} = \exp \left( -\frac{q^2}{4} \Delta r^2(t) \right) \).

For sufficiently small wavenumber \( q \) we observe sound waves in the intermediate scattering function \( F(q, t) \) and in the longitudinal current correlation function \( C_1(q, t) \). We determine their dispersion and damping. Temperature fluctuations are predicted to be either diffusive or nonhydrodynamic, depending on wavenumber and inelasticity as characterized by incomplete normal restitution.

12:27PM Q14.00007 Interparticle friction between gently contacting spheres, GREG FARRELL, NARAYANAN MENON, Dept of Physics, UMass Amherst. — In previous experimental work we have found that the packing fraction of gently-sedimented monodisperse spheres is affected by particle roughness as well as the viscosity and buoyancy provided by the surrounding fluid. In order to provide a macroscopic quantification of the microscopic effects of particle surface and of the fluid, we have developed a new technique to measure the coefficients of static and kinetic friction between two spheres in a fluid. We find that even in fluid environments, there are static and kinetic coefficients of friction characteristic of solid-on-solid contact. Surprisingly, even for a given pair of spheres, we measure a broad range of friction coefficients corresponding to contacts made at different locations on the surface. Thus, even for lubricated surfaces, surface heterogeneity is more apparent for small normal forces than at familiar force-scales.

1 Supported through NSF-DMR 0606216.

12:39PM Q14.00008 Spatial Force Correlations in 3D Granular Flow, NALINI EASWAR, KELSEY HATTAM, EFROSYNI SEITARIDOU, ALISA STRATULAT, Smith College, Northampton, MA., NARAYANAN MENON, University of Massachusetts, Amherst, MA. — We measure the force delivered at four locations on the boundary of a 3D flow of mono-disperse glass spheres in a vertical, cylindrical chute. A variable opening at the bottom is used to change the flow velocity \( v_f \) from 3 to 30 cm/s. The force is measured at 80KHz, allowing us to resolve individual collisions. We measure two-point spatial correlations in the flow direction and normal to it. The equal-time correlation between forces that are higher than a threshold shows a weak but measurable spatial correlation. This correlation shows no spatial directionality or dependence on flow rate. The time correlations are synchronous between diametrically opposed locations, and shifted in time between locations along the flow. From the time-lag we determine that the correlations are carried up the flow at speeds \( \sim 1000 v_f \). This speed increases as the flow approaches jamming.

1 Supported by NSF DMR 0606216 and NSF MRSEC DMR 0213695.

12:51PM Q14.00009 Impact phenomena in fluidized granular matter, PATRICK MAYOR, HIROAKI KATSURAGI, DOUGLAS DURIAN, University of Pennsylvania, Philadelphia — Projectiles dropped into granular media form a crater and come to rest in a particular way that has been actively investigated in numerous studies. These impact phenomena illustrate how particulate materials respond to externally applied forces. Several recent experiments have focused on the penetration of projectiles impacting granular materials at relatively low speeds, and measured the dynamics of the impact process, yielding force laws accounting for the observations. We present results showing how granular impacts are affected when the load on the grains is modified using a vertical gas flow. Balls or cylinders are dropped into a dry, noncohesive granular medium and we measure the penetration depth when gas is flown upward (thus unloading the contacts) or downward (loading the contacts). We observe that the frictional drag decreases linearly with the flow rate, and vanishes completely once the system is fluidized. Different projectile geometries allow us to separate the effect of normal and tangential frictional forces. We also consider the case of objects that are lowered quasi-statically into the granular medium and measure the net vertical force exerted by the granular system on the objects at each immersion depth. We then discuss how this resistance force compares with the forces observed in actual impacts experiments.

1:03PM Q14.00010 A Statistical Approach to the Filtration of Rods, SCOTT FRANKLIN, Rochester Institute of Technology — We investigate the efficacy of a square-grid mesh at filtering rods from solution. The volume fraction \( \phi \) is kept low, reducing the chance of rods cooperatively jamming at the mesh. For round particles, filtering at low \( \phi \) is trivially determined by the ratio of particle diameter to mesh size. Because rods have two length scales, filtering is non-trivial for meshes larger than the rod width but smaller than the length, a potentially very large range. We have measured experimentally the probability for a rod to be filtered as a function of mesh size, particle length, and aspect ratio. Results are compared with a theoretical extension of the Buffon-Laplace Needle problem that accounts for finite rod width and an isotropic distribution in the zenith angle. The solution is the probability that a spherocylinder in three dimensions makes contact with a 2D spherolithic mesh, a necessary but not sufficient condition for filtration. Comparison of experiment and theory is then suggestive of what conditions are both necessary and sufficient.

1 Supported in part by a grant from the National Science Foundation, Division of Materials Research.

1:15PM Q14.00011 Granular Breathing, SURAJIT SEN, ROBERT SIMION, SUNY-Buffalo, ADAM SOKOLOW, Duke University — We study the dynamics of monodispersed and tapered granular alignments held within a fixed boundary and a moving boundary. The system is assumed to be driven at one end by imparting a constant or time dependent acceleration to the edge grain. Analytical and simulational studies show that such a driven system can eventually get "over-compressed" and begin to dilate due to repulsive grain-grain interactions. Continuous driving results in the phenomenon of granular breathing. The talk shall discuss the dynamical processes associated with granular breathing for time-independent and time-dependent driving. The phenomenon of nonlinear resonance and related processes that arise in these systems will be discussed.

1 Research Supported by Army Research Office

1:27PM Q14.00012 Combustion of Micropowdered Biomass, ETHAN GEL, ROBERT THORNE, Cornell University — Combustion of finely powdered biomass has the potential to replace heating oil, which accounts for a significant fraction of US oil consumption, in heating, cooling and local power generation applications. When ground to 30-150 micron powders and dispersed in air, wood and other biomass can undergo deflagrating combustion, as occurs with gaseous and dispersed liquid fuels. Combustion is very nearly complete, and in contrast to sugar/starch or cellulose-derived ethanol, nearly all of the available plant mass is converted to usable energy so the economics are much more promising. We are exploring the fundamental combustion science of biomass powders in this size range. In particular, we are examining how powder size, powder composition (including the fraction of volatile organics) and other parameters affect the combustion regime and the combustion products.
both near and away from any critical point. Specifically, it has been shown that all thermodynamic observables of the p-state Potts model on a square lattice, MIKAEL WOOD, CARLOS WEXLER, University of Missouri — It has been recently discovered [1] that some families of systems exhibit universal behavior

[1] Partially supported by Fondecyt 1060317 and ICM P06-022-F.

11:27AM Q15.00002 An Efficient Numerical Approach for Nonlinear Fokker-Planck equations

11:39AM Q15.00003 Universal formulation of Casimir forces for static objects with arbitrary shapes and susceptibilities

11:51AM Q15.00004 Triggering and control of stick-slip friction

12:03PM Q15.00005 Topological order and topological memories at finite temperature

12:27PM Q15.00007 Extended Universality in Potts Models on Square and Triangular Lattices

12:39PM Q15.00008 Enhanced Transition Matrix Methods\textsuperscript{1}, DAVID YEVICK, University of Waterloo, MICHAEL REIMER, University of Waterloo — Recently we have adapted the transition matrix Monte-Carlo method to general communication systems [IEEE Photon. Technol. Lett. 1529 (2007), IEEE Communications Letters, 755 (2008)]. In these studies we compared and integrated different multicanonical and transition-matrix methods. We determined that the standard multicanonical method can be reformulated more simply and accurately by constructing the intermediate probability density function (density of states) after a small number of Markov transitions from the ratios of the elements of the transition matrix between adjacent states. Further, we considered an algorithmically more simple procedure in which transitions only occur from a given state to another state that has previously been less frequently sampled. Here we found that the intermediate Markov transition is small, numerical accuracy can be restored by restricting the Markov chain to within a single histogram bin for a certain number of transitions before allowing transitions to other bins. We finally summarize our application of these procedures to several problems in optical and wireless communication theory.

\textsuperscript{1}Funding for this work was provided in part by NSERC and Nortel.

12:51PM Q15.00009 S-index: Measuring significant, not average, citation performance, MANOLIS ANTONOYIANNAKIS, (1) Physical Review Letters, (2) Columbia University, (3) European Research Council — We recently [1] introduced the “citation density curve” (or cumulative impact factor curve) that captures the full citation performance of a journal: its size, impact factor, the maximum number of citations per paper, the relative size of the different-cited portions of the journal, etc. The citation density curve displays a universal behavior across journals. We exploit this universality to extract a simple metric (the “S-index”) to characterize the citation impact of “significant” papers in each journal. In doing so, we go beyond the journal impact factor, which only measures the impact of the average paper. The conventional wisdom of ranking journals according to their impact factors is thus challenged. Having shown the utility and robustness of the S-index in comparing and ranking journals of different sizes but within the same field, we explore the concept further, going beyond a single field, and beyond journals. Can we compare different scientific fields, departments, or universities? And how should one generalize the citation density curve and the S-index to address these questions? [1] M. Antonoyiannakis and S. Mitra, “Is PRL too large to have an ‘impact’?”, Editorial, Physical Review Letters, December 2006.

1:03PM Q15.00010 ABSTRACT WITHDRAWN —

1:15PM Q15.00011 Statistical laws for career longevity, ALEXANDER PETERSEN, WOO-SUNG JUNG, Boston University, JAE-SUK YANG, Korea University, H. EUGENE STANLEY, Boston University — Career length distinguishes successful long tenures from unsuccessful short stints, and partially reflects the contributions of an employee to the goals of the employer. In some professions, there are well-defined metrics that quantify career longevity, prowess, and productivity, which together contribute to the overall success rating for an individual employee. In this talk, I motivate a stochastic model for career development that relies on two key ingredients, random progress within the career and random stopping times terminating the career. This model is exactly solvable, predicting the probability density function (pdf) of career longevity, characterized by two parameters, $\alpha$ and $x_c$. The parameter $\alpha$ quantifies the power-law scaling of the pdf, which is terminated by an exponential cutoff after a crossover value $x_c$, representing the mean career lifetime. We test the model with the large quantity of empirical data available for several professional sports leagues, American baseball, Korean baseball, American basketball, and English soccer, finding excellent agreement with the model’s predictions. In all, the generality of the model suggests that there may be common stochastic forces that underly progress, success, and longevity in various professions.

1:27PM Q15.00012 Battles: Intelligent Army versus Insurgency\textsuperscript{1}, LINDA SHANAHAN, SURAJIT SEN, SUNY-Buffalo — A “simple” battle can be thought of as a conflict between two parties, each with finite reserves, and typically fought on one sides territory. Modern battles are often strategic, based largely on the speed of information processing and decision making and are mission oriented rather than to annex new territory. Here, we analyze such battles using a simple model in which the "blue" army fights a strategic battle against a "red" army that is well matched in combat power and in reds territory. We assume that the blue army attacks strategically while the red army attempts to neutralize the enemy when in close enough proximity, implemented here as "on-site," with randomly varying force levels to potentially confuse and drive the blue’s strategies. The temporal evolution of the model battles incorporate randomness in the deployment of the reds and hence possess attendant history dependence. We show that minimizing risk exposure and making strategic moves based on local intelligence are often the deciding factors that determine the outcome of battles among well matched adversaries.

\textsuperscript{1}Research Supported by th Army Research Office

1:39PM Q15.00013 Complete trails of social network evolution: The past 10 years of complex network research, DEOKJAE LEE, Seoul National University, KWANG-IL GOH, Korea University, BYUNGNAM KAHNG, DOOCHUL KIM, Seoul National University — During the last 10 years since the publication of pioneering papers on small-world and scale-free networks, more than 5,500 distinct researchers produced more than 4,000 research papers on complex networks during the years 1998–2007, here we study the complete evolution of the co-authorship network in network science. This dataset allows us to study the complete trail of social network evolution from the inception, in particular in the early transient stage, which has not been addressed empirically in previous studies. We find that distinct patterns in network topology emerge during the evolution: A fractal, tree-like giant cluster forms and in reds territory. We assume that the blue army attacks strategically while the red army attempts to neutralize the enemy when in close enough proximity, implemented here as “on-site,” with randomly varying force levels to potentially confuse and drive the blue’s strategies. The temporal evolution of the model battles incorporate randomness in the deployment of the reds and hence possess attendant history dependence. We show that minimizing risk exposure and making strategic moves based on local intelligence are often the deciding factors that determine the outcome of battles among well matched adversaries. In some professions, there are well-defined metrics that quantify career longevity, prowess, and productivity, which together contribute to the overall success rating for an individual employee. In this talk, I motivate a stochastic model for career development that relies on two key ingredients, random progress within the career and random stopping times terminating the career. This model is exactly solvable, predicting the probability density function (pdf) of career longevity, characterized by two parameters, $\alpha$ and $x_c$. The parameter $\alpha$ quantifies the power-law scaling of the pdf, which is terminated by an exponential cutoff after a crossover value $x_c$, representing the mean career lifetime. We test the model with the large quantity of empirical data available for several professional sports leagues, American baseball, Korean baseball, American basketball, and English soccer, finding excellent agreement with the model’s predictions. In all, the generality of the model suggests that there may be common stochastic forces that underly progress, success, and longevity in various professions.

1:51PM Q15.00014 Statistical mechanics of image processing by digital halftoning\textsuperscript{1}, JUN-ICHI INOUE, WATARU NORIMATSU, Hokkaido University, YOHEI SAIKA, Wakayama NCT, MASATO OKADA, The University of Tokyo — We consider the problem of digital halftoning (DH). The DH is an image processing representing each grayscale in images in terms of black and white dots, and it is achieved by making use of the threshold dither mask, namely, each pixel is determined as black if the grayscale pixel is greater than or equal to the mask value and as white vice versa. To determine the mask for a given grayscale image, we assume that human-eyes might recognize the BW dots as the corresponding grayscale by linear filters. Here we found that while substantial errors often result if the perturbation in the link, adjacent Markov state is small, numerical accuracy can be restored by restricting the Markov chain to within a single histogram bin for a certain number of transitions before allowing transitions to other bins. We finally summarize our application of these procedures to several problems in optical and wireless communication theory.

\textsuperscript{1}We acknowledge Grant-in-Aid Scientific Research on Priority Areas “Deepening and Expansion of Statistical Mechanical Informatics (DEX-SMI)” No. 18079001.
2:03PM Q15.00015 Molecular Kinetic Analysis of a Finite-Time Carnot Heat Engine, YUKI IZUMIDA, KOJI OKUDA, Hokkaido University — We show the first derivation of the efficiency at the maximum power for a finite-time Carnot heat engine of a weakly interacting gas which we can regard as a nearly ideal gas. Using this simple model, we check the celebrated Curzon-Ahlborn (CA) efficiency by performing the event-driven MD simulation as a numerical experiment for the first time[1,2]. This numerical experiment reveals that the CA efficiency is realized only in the limit of the small temperature difference \( T_L \rightarrow T_H \), where \( T_L \) and \( T_H \) are the temperatures of the hot and cold heat reservoirs, respectively. Our molecular kinetic analysis can explain the numerical results theoretically.


Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q16 DAMOP: Focus Session: Dipolar Gases and Ultra-Cold Molecules 317

11:15AM Q16.00001 Novel quantum magnets: Dipolar quantum gases1, HAN PU, Rice University — Experimental creation of chromium condensate with large magnetic dipole moment and ultracold polar molecules with large electric dipole moment has generated significant interest in dipolar quantum gases. The long-range and anisotropic nature of the dipolar interaction potential greatly enriches the properties of the system, many of which are not present in their non-dipolar counterparts. In this talk, I will present our recent studies on dipolar BEC as well as dipolar fermions, with the emphasis on the latter which is relatively less studied. From a semi-classical calculation based upon the phase space representation of the Fermi gas, I will show how the dipolar interaction deforms the Fermi surface and manifests itself in collective excitations and time-of-flight expansion dynamics of the cloud. Finally, I will describe a self-consistent Hartree-Fock-Bogoliubov theory that also takes dipolar induced fermionic superfluid pairing into account.

1Support from NSF and the Robert A. Welch foundation is acknowledged.

11:51AM Q16.00002 Ultracold Heteronuclear Fermi-Fermi Molecules, KAI DIECKMANN, Ludwig-Maximilians-University of Munich, Germany — Spin mixtures of quantum-degenerate fermionic gases exhibit long lifetimes in the strongly-interacting regime near a Feshbach resonance. This has opened the door for numerous key experiments like the creation of Fermi-Fermi molecules, the realization of molecular BEC, the observation of a pairing gap and of superfluidity in a fermionic gas in the BEC-BCS cross-over region near a Feshbach resonance. We present the production of \(^{6}\text{Li}-^{40}\text{K}\) heteronuclear molecules based on our experimental platform for the production of a two-components mixture of quantum-degenerate Fermi gases. Our production scheme for quantum-degenerate fermionic \(^{6}\text{Li}\) and \(^{40}\text{K}\) and bosonic \(^{87}\text{Rb}\) gases is based on multiple species magneto-optical trapping [1] and sympathetic cooling of the fermions by rubidium. We demonstrated catalytic cooling of lithium by potassium, overcoming the small lithium rubidium cross section. We achieved to simultaneously enter quantum degeneracy for all three species [2] with lowest temperatures of 0.25 and 0.35 times the Fermi temperature for lithium and potassium at about 260 nK. The highest atom numbers achieved are \(1.8 \times 10^5\) for lithium as well as potassium, and about \(1 \times 10^5\) for rubidium. We studied two s-wave Feshbach resonances between lithium and potassium [3] at 155 G and 168 G. By magnetic field sweeps we created about \(4 \times 10^{46}\) \(^{6}\text{Li}-^{40}\text{K}\) molecules at conversion efficiencies of up to 50% [4]. With a Stern-Gerlach purification technique we are able to image molecules and atoms spatially separated from each other. We discuss the lifetime of the molecule-atom mixture close to resonance.

References:

12:27PM Q16.00003 Quantum phases of a two-dimensional dipolar Fermi gas, GEORG BRUUN, Niels Bohr Institute, EDWARD TAYLOR, Universita di Trento — We examine the superfluid and collapse instabilities of a quasi two-dimensional gas of dipolar fermions aligned by an orientable external field. It is shown that the interplay between the anisotropy of the dipole-dipole interaction, the geometry of the system, and the dipole polarization of the superfluid order parameter means that the effective interaction for pairing can be made very large without the system collapsing. This leads to a broad region in the phase diagram where the system forms a stable superfluid. Analyzing the superfluid transition at finite temperatures, we calculate the Berezinskii–Kosterlitz–Thouless temperature as a function of the dipole angle.

12:39PM Q16.00004 Fermi surface distortions in a neutral Fermi fluid with dipolar interactions, BENJAMIN M. FREGOSO, UIUC, KAI SUN, EDUARDO FRADKIN, BENJAMIN LEV — We show that the Fermi surface of a neutral fluid of fermions with aligned dipole moments by an external field is elongated along the direction of the aligning field. The distortion of the Fermi surface can be expressed as a linear combination of Legendre polynomials \( P_l(k) \) with \( l = \text{even} \), with \( l = 2 \) being the leading term. The possible existence of a phase transition to a spontaneous biaxial phase is discussed. The zero- sound collective modes of the system are found to be strongly anisotropic. We discuss the possible use of light scattering experiments to detect spatial anisotropies in dipolar gases.

12:51PM Q16.00005 Devil’s staircase and supersolidity in one-dimensional dipolar Bose gases, S. L. SONDHI, F. J. BURNELL, MEERA M. PARISH, Princeton University, N.R. COOPER1, Cambridge University — The classical ground states of particles in a convex repulsive potential are known to have a phase portrait displaying a complete devil’s staircase structure. We consider a single- component gas of dipolar bosons confined in a one-dimensional optical lattice, where the dipoles are aligned such that the long-ranged dipolar interactions are maximally repulsive. Introducing a kinetic term tunes the system away from the classical limit and results in a phase diagram with a Mott- Hubbard lobe for each rational filling fraction. Tuning the on-site interaction away from convexity yields alternative commensurate states with double occupancies which can form a staircase of their own, as well as one dimensional "supersolids" which simultaneously exhibit discrete broken symmetries and superfluidity.

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10:30PM Q16.00006 Roton softening and supersolidity in Rb spinor condensates, ROBERT CHERNG, EUGENE DEMLER, Harvard University — Superfluids with a tendency towards periodic crystalline order have both a phonon and roton like spectrum of collective modes. The softening of the roton spectrum provides one route to a supersolid. We show that roton softening occurs in \(^{87}\text{Rb}\) spinor condensates once dipolar interactions and spin dynamics are taken into account. By including the effects of a quasi-two-dimensional geometry and rapid Larmor precession, we show a dynamical instability develops in the collective mode spectrum at finite wavevectors. We construct phase diagrams showing a variety of instabilities as a function of the direction of the magnetic field and strength of the quadratic Zeeman shift. Our results provide a possible explanation of current experiments in the Berkeley group Phys. Rev. Lett. 100,170403 (2008).
1:15PM Q16.00007 Hexatic, Wigner crystal and superfluid phases of dipolar bosons1. KAUSHIK MITRA, CARL WILLIAMS, NIST Gaithersburg, CARLOS SA DE MELO, Georgia Institute of Technology — The finite temperature phase diagram of two-dimensional dipolar bosons versus dipolar interaction is discussed for different values of short range repulsions. We identify the stable phases as superfluid, dipolar Wigner crystal (DWC), dipolar hexatic liquid crystal (DHL), and normal fluid. In particular, we show that the DWC exists at low temperatures for large dipolar interactions, but it melts into a DHL at higher temperatures, where translational lattice order is destroyed, but orientational order is preserved. Upon further increase in temperature the DHL phase melts into the normal fluid, where both orientational and translational lattice order are absent. We also find that the supersolid phase has always higher energy than the superfluid or Wigner crystal phases at low temperatures, but the supersolid is metastable, having an energy minimum that may be accessed through thermal quenching. Lastly, we calculate the static structure factor for each of the stable phases and show that each phase can be identified uniquely in an optical Bragg scattering experiment.

1Supported under ARO Award W911NF0710576 with funds from the DARPA OLE Program.

1:27PM Q16.00008 Dipole moments of ultra-cold polar molecules: a quantum Monte Carlo study, MICHAL BAJDICH, SHI GUO, LUBOS MITAS, CHIPS, Department of Physics, NC State, Raleigh, NC, PETER J. REYNOLDS, Physics Division and Physical Sciences Directorate, U.S. ARO, Durham, NC — Recently, there has been a great deal of interest in the production of ultra-cold heteronuclear molecules having large electric dipole moments [1]. This is of interest both for fundamental reasons as well as for applications such as qubits for quantum computing [2]. In this work, we calculate the dipole moment of a potentially implementable two-atom alkaline-alkaline-earth molecule, Li2Sr. We use correlated wave-function methods including both the quantum chemical configuration interaction (CI) method, and a stochastic quantum Monte Carlo (QMC), to calculate the potential energy surface and dipole moment. We study the dipole moment with increasing accuracy of correlated wave-functions. We then variationally re-optimize the wave-functions, which then serve as the representation of the Fermion nodes in the fixed-node QMC. To treat the Sr atom we employ two types of effective core potentials (ECPs), large core ECPs have only s-states in the valence space, while the small core ECP’s valence space includes also the highest s and p semi-core sub-shells. We find significant sensitivity of the dipole moment on both the size of the valence space and on the accuracy of the Fermion nodes. [1] B. Damski, et al Phys. Rev. Lett. 90, 110401 (2003). [2] D. DeMille, Phys. Rev. Lett. 88, 067901 (2002).

1:39PM Q16.00009 Using an optical lattice to preform KRb molecules and enhance the efficiency of ultra-cold polar molecule formation1, JAMES FREERICKS, Georgetown University, MACIEJ MASKA, University of Silesia, ROMUALD LEMANSKI, Institute for Low Temperature and Structure Research, THOMAS HANNA, National Institute of Standards and Technology, PAUL JULIENNE, Joint Quantum Institute of the University of Maryland and the National Institute of Standards and Technology — We will discuss recent computational work that employs both direct quantum Monte Carlo simulation and inhomogeneous dynamical mean-field theory to study the efficiency of preforming KRb pairs in an optical lattice. We will describe how to optimize the efficiency by adjusting the lattice depth and the interspecies interaction (via the Feshbach resonance) with parameters specific for fermionic 40K and bosonic 87Rb (since the ground-state dipolar molecule has already been formed from those atoms in free space). We work with a deep enough lattice that the K atoms are mobile, but the Rb atoms are localized, so the system is described by the spinless Falicov-Kimball model on a two-dimensional lattice. We also calculate the entropy and estimate the temperature turning the lattice.

1Supported under ARO Award W911NF0710576 with funds from the DARPA OLE Program.

1P16.00010 The bound states of ultracold KRb molecules, PAUL JULIENNE, Joint Quantum Institute, NIST and the University of Maryland. THOMAS HANNA, NIST — Recently ultracold vibrational ground state 40K40Rb polar molecules have been made using magnetoassociation of two cold atoms to a weakly bound Feshbach molecule, followed by a two-color optical STIRAP process to transfer molecules to the molecular ground state [1]. We have used accurate potential energy curves for the singlet and triplet states of the KRb molecule [2] with coupled channels calculations to calculate all of the bound states of the 40K40Rb molecule as a function of magnetic field from the cold atom collision threshold to the $\hbar\Omega=0$ ground state. We have also developed approximate models for understanding the changing properties of the molecular bound states as binding energy increases. Some overall conclusions from these calculations will be presented. [1] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Peer, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, Science, 2008, 322, 231–235. [2] A. Pashov, O. Docenko, M. Tamanis, R. Ferber, H. Knöckel, and E. Tiemann, Phys. Rev. A, 2007, 76, 022511.

2:03PM Q16.00011 Multichannel quantum defect theory model of Feshbach resonances, THOMAS HANNA, National Institute of Standards and Technology, EITE TIESINGA, PAUL JULIENNE, Joint Quantum Institute, NIST and University of Maryland — Multichannel quantum defect theory (MQDT) has a large number of applications in atomic physics, including the properties of collisions near threshold. The key concept is that the short range physics can be accounted for very simply and then matched to the asymptotic long range interaction. We have developed a model of Feshbach resonances based on the ideas of MQDT. This model allows calculation of the kinkel fields at which resonances occur, as well as properties such as the resonance width and background scattering length. Apart from known atomic properties, only three input parameters are required: the singlet and triplet scattering lengths, and the coefficient of the long range van der Waals potential. Analytic reference functions defined by the potential [1] are used to calculate the long range properties, which are linked to the short range physics through a frame transformation. We apply our theory to calculate all of the bound states of the 87KRb molecule [1]. We have used accurate potential energy curves for the singlet and triplet states of the KRb molecule [2] with coupled channels methods including both the quantum chemical configuration interaction (CI) method, and a stochastic quantum Monte Carlo (QMC), to calculate the potential energy surface and dipole moment. We study the dipole moment with increasing accuracy of correlated wave-functions. We then variationally re-optimize the wave-functions, which then serve as the representation of the Fermion nodes in the fixed-node QMC. To treat the Sr atom we employ two types of effective core potentials (ECPs), large core ECPs have only s-states in the valence space, while the small core ECP’s valence space includes also the highest s and p semi-core sub-shells. We find significant sensitivity of the dipole moment on both the size of the valence space and on the accuracy of the Fermion nodes. [1] B. Damski, et al Phys. Rev. Lett. 90, 110401 (2003). [2] D. DeMille, Phys. Rev. Lett. 88, 067901 (2002).
11:27AM Q17.00002 Lower limit on the achievable temperature in resonator-based sideband cooling

11:39AM Q17.00003 Strong single-qubit lasing and cooling at the symmetry point?

11:51AM Q17.00004 Two-level systems driven by large-amplitude fields

12:03PM Q17.00005 Quantum coherence in a Josephson junction array circuit.

12:15PM Q17.00006 Quantum information processing with a Josephson ring modulator.

12:27PM Q17.00007 1/f Flux Noise in SQUIDs and Josephson Junction Qubits

12:39PM Q17.00008 Josephson junction array protected from local noises.
Our result indicates that the entanglement between the two JVQs is significant. Also, we show that the concurrence of the JVQs, placed in a resonant potentials by using the instanton and the valley-instanton approaches, respectively. We compute the concurrence to estimate the level of entanglement of two potential and leads to the interaction between the qubits. We compute the MQT of the fluxons between the minima of the symmetric and asymmetric double-well DHUNGANA, ISAAC O'BRYANT, JU KIM, University of North Dakota — We discuss the entanglement of two Josephson vortex qubits (JVQs) interacting by the continuous charge term, while the Davidson type affects the discrete charge term. These properties are linked to the boundary conditions of these systems.

The loss mechanisms are likely to be important for understanding coherence times in Josephson qubit circuits. The two-level systems (TLSs) naturally occurring in Josephson junctions constitute a major obstacle for the operation of superconducting phase qubits. Since these TLSs can possess remarkably long decoherence times, we show that such TLSs can themselves be used as qubits, allowing for a well controlled initialization, universal sets of quantum gates, and readout. Thus, a single current-biased Josephson junction (CBJJ) can be considered as a multiqubit register. It can be coupled to other CBJJs to allow the application of quantum gates to an arbitrary pair of qubits in the system. We also show that using the dynamics of a driven qubit, it could serve as a hallmark of coherent quantum dynamics in ladder-like multilevel systems. A real-space implementation of the quantum walk may help to verify qubits coupled to high quality resonators. The quantized behavior stands in contrast with the smooth dependence expected for a classical random walk, and distinguished by a winding number defined in terms of the Bloch eigenstates in the Brillouin zone. We find that the mean displacement of a particle initially localized on one of the two sublattices. The corresponding non-Hermitian tight-binding problem with complex potential for the decaying sites exhibits two distinct phases, distinguished by a winding number defined in terms of the Bloch eigenstates in the Brillouin zone. We find that the mean displacement of a particle initially localized on one of the two sublattices.

质子和超导线路的量子态和拓扑统计特性

1:03PM Q17.00010 Controllable scattering of photons in a one-dimensional resonator waveguide

1:15PM Q17.00011 Quantum two-level systems in Josephson junctions as naturally formed qubits

1:27PM Q17.00012 Topological states and braiding statistics using quantum circuits

2:03PM Q17.00015 Entanglement of Two Josephson Vortex Qubits in Resonant Cavity

2:15PM Q17.00016 Two Types of Loss Expected for Josephson Qubit Circuits

3:00PM Q17.00017 Dynamics of Josephson Junctions and Superconductivity

Wednesday, March 18, 2009 11:15AM - 2:15PM – Session Q18 DPOLY: Theory and Simulation I
11:15AM Q18.00001 Design of Thermoplastic Elastomers with Self-Consistent Mean Field Theory: Radial (ABA)\textsubscript{n} and A(ABA)\textsubscript{n} Miktoarm Architectures, NATHANIEL LYND, FULUSHO OYEROKUN, DONAL O’DONOGHUE, Department of Chemical Engineering and the Materials Research Laboratory, University of California, Santa Barbara — Two thermoplastic elastomer designs were evaluated using self-consistent mean field theory. The phase diagram of a radial (A\textsubscript{1}B\textsubscript{2})\textsubscript{n} block copolymer was calculated at $\chi N = 40$ per arm as a function of composition ($f_A$) and asymmetry between the A-end blocks ($\tau = N_{A1}/(N_{A1} + N_{A2})$). Significant deflection of the phase boundaries towards larger $f_A$ occurred for asymmetric triblock copolymers ($\tau \approx 0.15$ and $\tau \approx 0.90$) due to the interplay between bidispersity and chain-pullout of the A-blocks. The phase diagram of an A\textsubscript{1}(B\textsubscript{2}A\textsubscript{2})\textsubscript{n} miktoarm star triblock copolymer was also investigated as a function of $f_A$ and $\tau$ at $\chi N = 40$ per A\textsubscript{1}B\textsubscript{2} unit. Similar deflections in phase boundaries towards higher $f_A$ resulted.

11:27AM Q18.00002 Unified mathematical model for linear viscoelastic predictions of linear monodisperse and polydisperse and branched polymers, RENAT KHALILLIIN, JAY SCHIEBER — We present an application of a single-chain mean-field model for entangled linear blends and star-branched systems. Slip-links instead of tubes are employed. The entanglements on a chain are destroyed by two coupled relaxation processes: so-called sliding dynamics; and relaxation of the environment, so-called constraint dynamics. The constraint dynamics are implemented by destruction and creation of the entanglements in the middle of the chain in a way statistically self-consistent with sliding dynamics. In contrast to previous tube models, Rouse dynamics is completely avoided. Nonetheless, the implementation of constraint dynamics in tube models is different for linear and branched chains; the slip-link model shows no need for modification of constraint dynamics. Moreover, our slip-link model requires a single fitting parameter $\chi N K$, that depends on the temperature of the melt, but not on chain length. The parameter can be fixed from a single fit to linear viscoelastic data. In addition, for branched polymers the branch point movements are determined by the free energy, so that its position is allowed to fluctuate, and even slide through the slip-links. The resulting model exhibits primitive-path fluctuations and chain stretching, so could be applied to flow and generalized to more complicated branches or cross-linked networkswithout significant modifications.

11:39AM Q18.00003 Self-assembly of rod coil block copolymers under confinement, MANAS SHAH, VENKAT. GANESAN, The University of Texas at Austin — The interplay of microphase separation and liquid crystalline ordering in rod-coil block copolymers leads to formation of complex morphologies distinct from that of conventional flexible block copolymer phases. In order to be used for organic electronic applications such as photovoltaic cells, rod-coil block copolymers must be patterned into thin films. The final morphology and the nature of orientation of rod units would be determined by the interplay between the interactions on the interactions of the blocks with the confining surfaces. We combine the self-consistent field theory models of rod-coil block copolymers in a thin film framework to understand the effect of confinement on the morphology and the nature of orientation of rod-units. Also for nearly symmetric rod-coil copolymers, we analyze the parallel – perpendicular lamellae transitions using a free energy framework. Also, we consider morphologies of such block copolymers (and blends) which can be utilized for higher device efficiency in photovoltaic cells.

11:51AM Q18.00004 Theoretically Informed Particle-Based Simulations of Polymers in Arbitrary Ensembles, DARIN PIKE, FRANCOIS DETCHEVERRY, University of Wisconsin, MARCUS MUELLER, University of Goettingen, JUAN DE PABLO, University of Wisconsin — A new, particle-based formalism is proposed for simulation of polymeric materials, where the interaction energy is given by the standard functional employed in field-theoretic models. The main features of the proposed formalism reside in its ability to enable simulations at constant stress or constant pressure, thereby permitting accurate estimation of free energies and phase boundaries. The usefulness of the proposed approach is illustrated in a series of thermodynamic property calculations from Monte Carlo simulations in the nVT, nPT, semi-grandcanonical and Gibbs ensembles. In particular, we consider the phase separation of a binary homopolymer blend and a symmetric diblock copolymer. For the blend, we present results for the phase diagram and the critical point of the model. For symmetric copolymers, we study the distribution of local stress in lamellae and the location of the first-order transition from a disordered to a lamellar phase.

12:03PM Q18.00005 Fields Help Particles – Fast Off-Lattice Monte Carlo Simulations of Soft Materials, YUHUA YIN, QIANG WANG, Colorado State University — Conventional molecular simulations of multi-chain systems are hindered by “hard” excluded-volume interactions (e.g., the Lennard-Jones potential in off-lattice simulations and the self- and mutual-avoiding walks in lattice simulations). Although such interactions are necessary for obtaining realistic dynamics, they significantly slow down the chain relaxation towards equilibrium configurations and efficient sampling of the configurational space. The idea of fast off-lattice Monte Carlo (FOMC) simulations is to perform particle-based Monte Carlo simulations in continuum with a Hamiltonian commonly used in polymer field theories, where individual polymer segments are modeled as “soft” particles whose interaction energy is finite when they overlap. This leads to much faster chain relaxation and better sampling of the configurational space. Furthermore, using the same Hamiltonian in both polymer field theories and FOMC simulations enables quantitative comparisons between them without any parameter-fitting to unambiguously reveal the effects of fluctuations and correlations in the system. Here we demonstrate these great advantages of FOMC simulations using several model systems.

12:15PM Q18.00006 Particles vs. Fields – Finite-Range Interactions in Polymer Field Theories, QIANG WANG, Colorado State University — Recently, we proposed a particle-based, fast off-lattice Monte Carlo (FOMC) simulation that uses the same Hamiltonian as in polymer field theories, which has great advantages over conventional molecular simulations. However, the continuous Gaussian chain model and $\delta$-function interactions widely used in polymer field theories (such as the self-consistent field theory) cannot be directly used in FOMC simulations. We therefore extend the field theories to the discrete Gaussian chain model and finite-range interactions. Taking the microphase separation of diblock copolymers as an example, a finite range interaction range increases the order-disorder transition from the well-known result of $\chi N \approx 10.5$, as well as the bulk lamellar period. More importantly, this work allows direct comparisons between the polymer field theories and FOMC simulations without any parameter-fitting to unambiguously and quantitatively reveal the effects of fluctuations and correlations in the system.

12:27PM Q18.00007 Mean Field Theory for Ionomer Melts, ERICA SALZTMAN, SANAT KUMAR, Columbia University — Single Chain Mean Field theory is applied to melts of charged polymers. Control parameters include temperature, chain length, and monomer density. Equilibrium variations of polymer conformational, translational, and rotational degrees of freedom and counterion translational degrees of freedom are studied; in particular we are interested in conformational and morphological transitions which occur in ionomers with changes in temperature and apparently dominate their macroscopic behavior. The constituent interactions, which are compared to simulation findings of low temperature condensation of chains and counterions to form ordered sheets of charges, form the basis for stochastic theories which model the temporal evolution of these structures, with immediate relevance to measurable dynamic properties.
12:39PM Q18.00008 Equilibrium and Beyond Equilibrium Properties of Polyelectrolytes - Ewald-Like Approach for Fluctuating Hydrodynamic and Electrostatic Interactions

JUAN P. HERNANDEZ-ORTIZ, Department of Materials, Universidad Nacional de Colombia, Sede Medellín, MICHAEL D. GRAHAM, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — A method is proposed for self-consistent simulations of the equilibrium and beyond equilibrium structures and transport properties of polyelectrolytes in solution. The method incorporates solution of the Nernst-Planck diffusion equation for ions and counter-ions within the solvent, and simultaneous description of fluctuating hydrodynamic interactions by means of a Green’s function formalism. The proposed approach generalizes our $\mathcal{O}(N)$ general geometry Ewald-like method to simultaneous treatment of hydrodynamics and electrostatics. With this method, we examine the transport properties of polyelectrolytes solutions at rest and in various flow fields, and we make direct comparisons to results from explicit ion Brownian dynamics simulations and experimental observations.

12:51PM Q18.00009 Self Consistent Field Theory Study of the Effect of Grafting Density on the Height of a Weak Polyelectrolyte Brush

KEVIN WITTE, YOU-YEON WON, Purdue University — The height of weakly basic polyelectrolyte brushes in the osmotic brush regime is studied as a function of the grafting density using a numerical self-consistent field (SCF) theory derived from the (semi-) grand canonical partition function. The theory is shown to properly account for the local nature of the charge equilibrium and to be able to capture the basic behaviors of polyelectrolyte brushes, including brush height variation with salt concentration and scaling with respect to degree of polymerization. However, we find, in agreement with recent experiments, that the scaling of brush height with grafting density is qualitatively different than that predicted by basic scaling arguments. This difference is attributed to the relative strength of electrostatic type interactions compared to finite segment size packing constraints.

1:03PM Q18.00010 Adsorption and depletion of polyelectrolyte in charged

DADONG YAN, XINGKUN MAN, State Key Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, Chinese Academy of Sciences, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University, NSFC COLLABORATION — Self-consistent field theory is presented to study the adsorption of flexible polyelectrolyte brushes (PE) onto uniformly oppositely charged cylinders. We focus on the curvature effect of adsorbing surface on the adsorption-depletion phase transition-like behavior. In terms of the scaling expression of the critical quantities, i.e., the salt concentration, the charge fraction of PE chain and the area density of surface charge, at the adsorption-depletion transition point have been obtained. Moreover, we find a critical line for the dependence of the critical radius of cylinder on the salt concentration, which separates the adsorption and depletion states. The theoretical results are in good agreement with the Monte Carlo simulations and the experimental results.

1:15PM Q18.00011 Field-Based Modeling and Simulation of Interfacial Fluctuations in Block Copolymers

AUGUST BOSSE, Polymers Division, NIST — The Edwards-model-based, field-theoretic simulation framework of Fredrickson is the cutting edge methodology in coarse-grained, field-based simulation of fluctuating copolymer systems [V. Ganesan and G.H. Fredrickson, Europhys. Lett. 55, 814 (2001); G.H. Fredrickson, V. Ganesan, and F. Drolet, Macromolecules 35, 16 (2001)]. Coarse graining the standard Edwards model yields the classic phenomenological “phase field” model of Ohta and Kawasaki [T. Ohta and K. Kawasaki, Macromolecules 19, 2621 (1986)]. Further coarse graining, coupled with the assumption of weak segregation, yields the ubiquitous Leibler-Brazovskii-Fredrickson-Helfand model [G.H. Fredrickson and E. Helfand, J. Chem. Phys. 87, 697 (1987)]. Each of these field-based models is capable of capturing thermodynamic fluctuations; however, the applicability of each model depends on the quench depth, the molecular weight, and the composition of the constituent copolymers, among other variables. Here we examine fluctuation effects in, and limitations of field-based models in the context of measuring interfacial fluctuations in a two dimensional diblock copolymer melt.

1:27PM Q18.00012 Variational Coarse-Graining of Discretized Field Theories of Fluids

MICHAEL VILLET, GLENN FREDRICKSON, University of California, Santa Barbara — Statistical field theory models have proven to be valuable tools for studying the equilibrium behavior of polymeric fluids, but direct simulation of these field theories without use of the mean field approximation is computationally demanding. Computational resources can be extended to simulate larger systems by discretizing the field variables with a coarsely spaced lattice, but indelicate coarse graining risks truncation of important short-wavelength physics. We introduce a variational method for systematically coarse-graining discretized field theoretic models of fluids while minimizing this truncation error.

1:39PM Q18.00013 Simulation of Fluctuations in Diblock Copolymer Melts: Testing an Alternative to the Fredrickson-Helfand Theory

JIAN QIN, CEMS at Universiy of Minnesota, DAVID MORSE, CEMS at University of Minnesota — Simulations of a bead-spring model of disordered diblock copolymer melts have been conducted to test a renormalized one-loop (ROL) theory of composition fluctuations recently proposed by the authors. The simulations use hybrid Monte Carlo (MC) / Molecular Dynamics (MD), reptation and double-rebriding moves, combined with replica exchange, to relax chain conformations. The quantitative comparison of simulation results with theory relies on a procedure that uses perturbation theory to independently identify the self-consistent-field (or RPA) interaction parameter. For the modest chain lengths accessible to simulations ($N \leq 64$ here), results for the maximum $S(q^*)$ of the structure factor are quite different from both RPA and Fredrickson-Helfand predictions, but agree very well with renormalized one-loop predictions.

1:51PM Q18.00014 Microphase Separation Induced by the Differential Monomer-Monomer Interactions in Diblock Copolymer/Homeopolymer Blends

JIAJIA ZHOU, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University — Phase diagrams of blends composed of diblock copolymer (AB) and homopolymer (C) are obtained using the random phase approximation and self-consistent field theory. Emphasis is placed on the special case where all three monomer pairs, A/B, B/C and C/A, are miscible. Despite the miscibility of the binary pairs, a close-loop immiscible region exists in the AB/C blends when the pair interaction parameters are sufficiently different. Inside the close-loop, the system undergoes microphase separation, exhibiting different morphologies. This phenomenon is enhanced when the homopolymer interacts much strongly to one of the blocks of the diblock copolymer. The theoretical results are used to explain some recent experiments.
2:03PM Q18.00015 Study on the strength of intermonomer interactions for PS-b-PMMA using compressible RPA. HYUNJUH AHN, DU YEOL RYU, Yonsei University, YOUNGMIN KIM, Hongik University, KWANG HYUN SONG, KYUNG WOOK KWON, JUNHAN CHO, Dankook University — PS-b-PMMA copolymer is one of the most useful nanoscopic materials that can be used as passive electronic materials, and also as templates and scaffolds. It is then clear that the better knowledge on the strength of intermonomer interactions for the PS-b-PMMA is of great importance in fabricating nanomaterials from it. Using a compressible random-phase approximation (RPA) theory, we discuss mainly the second-order vertex function in the compressible Landau free energy. This vertex function is involved in the exchange energy between self and cross interactions along with the self interaction difference. Ordering transition temperatures are predicted and compared with experimental measurements using small-angle X-ray scattering (SAXS) and depolarized light scattering. A close relationship between barotropy (ordering upon pressurization) and the energetic vertex term for the copolymer is argued. 1

We feel grateful for the support from Center for Photofunctional Energy Materials.

Wednesday, March 18, 2009 11:15AM - 2:15PM —
Session Q19 DPOLY: The Physics of Polymer Nanocomposites: Rheology and Mechanical Properties 320

11:15AM Q19.00001 Influence of Nanoparticles on the Amplitude of Molecular Motions and the Fragility a Model Glass-Forming Polymer Melt. , JACK DOUGLAS, polymers Division, National Institute of Standards and Technology, FRANCIS STARR, Department of Physics, Wesleyan University — We investigate the impact of the addition of nanoparticles on both the fast and slow dynamics of a coarse-grained polymer fluid by molecular dynamics. The fast dynamics is characterized by the Debye-Waller factor (the average mean square particle displacement at a characteristic time in the caged particle motion regime) and the slow structural relaxation is characterized by the coherent intermediate scattering function. Our study explores how both the polymer-particle and nanoparticle volume fraction change the amplitude of the high frequency molecular motions (relative to the pure melt reference condition) and the strength of the temperature dependence of the structural relaxation time (defining the fragility of glass formation, as well as the glass transition temperature). Substantial variations of the Debye-Waller factor are observed and we test the effectiveness of the Buchenau relation linking the Debye-Waller factor to the long time structural relaxation time. We also consider how the presence of nanoparticles in the polymer melt influence the fragility of glass formation, where a range of criteria are utilized to define fragility. Appreciable changes of fragility are observed, these changes being dependent on the nanoparticle concentration and particle-polymer interaction.

11:27AM Q19.00002 Macroscopic dynamics of polystyrene grafted silica nanoparticles in a homopolymer matrix. JOSEPH MOLL, Columbia University, PINAR AKCORA, University of Missouri, SANAT KUMAR, Columbia University, RALPH COLBY, Pennsylvania State University — Silica nanoparticles grafted with polymers, dispersed in a homopolymer matrix, and annealed over time adopt a broad range of dispersion states which depend on grafting density, annealing time, weight percent silica, and the molecular weights of the polymers. We tuned these variables to give desired dispersion states, from uniformly dispersed particles to agglomerated clusters. Rheology was used to critically determine how the dispersion state affects the mechanical reinforcement of the composite. We have run both steady shear and small amplitude oscillatory shear experiments on nanocomposites comprising a range of dispersion states. By mapping the observed reinforcement on a morphology diagram, we observe the location of a maximum in reinforcement.

11:39AM Q19.00003 Structure, ion transport and rheology of nanoparticle organic hybrids. HAIQO QI, LYNDEN ARCHER, Cornell University — We report a new class of liquid nanoparticle organic hybrid materials (NOHMs), produced by tethering an organic oligomer corona to the surface of inorganic nanoparticles, and investigate their use as electrolytes. This talk focuses on the structure factor and the dispersion state affects the mechanical reinforcement of the composite. We have run both steady shear and small amplitude oscillatory shear experiments on nanocomposites comprising a range of dispersion states. By mapping the observed reinforcement on a morphology diagram, we observe the location of a maximum in reinforcement.

11:51AM Q19.00004 Effect of filler surface properties on stress relaxation behavior of carbon nanofiber/polyurethane nanocomposites. I. SEDAT GUNES, GUILLERMO JIMENEZ, SADHAN JANA, The University of Akron — The effect of carbon nanofiber (CNF) surface properties on tensile stress relaxation behavior of CNF/polyurethane (PU) nanocomposites was analyzed. PU was synthesized from methane diisocyanate, polypropylene glycol (PPG diol), and butanediol. CNF, oxidized CNF (ox-CNf), and PPG diol grafted CNF (ol-CNf) were selected as fillers. ol-CNf was obtained by grafting PPG diol onto ox-CNf by reacting it with the carboxyl groups present on ox-CNf surface. The atomic ratios of oxygen to carbon present on the filler surfaces were 0.13 and 0.18 on ox-CNf and on ol-CNf as compared to 0.015 on CNF, mostly due to the presence oxygen containing polar groups on the surfaces of the former. The composites were prepared by in-situ polymerization and melt mixing in a chaotic mixer. The stress relaxation behavior of composites was determined at room temperature after inducing a tensile strain of 100%. The presence of fillers augmented the rate of stress relaxation in composites which was highest in the presence of CNF. The results suggested that relatively weak polymer-filler interactions in composites of CNF promoted higher stress relaxation.

12:03PM Q19.00005 Synthesis of metal-molecule-metal structures for single-molecule transport and spectroscopy measurements. ALEX NEUHAUSEN, Dept. of Electrical Engineering, Stanford University, DAVID GOLDHABER-GORDON, Dept. of Physics, Stanford University, CHRIS CHIDSEY, Dept. of Chemistry, Stanford University — Robust, repeatable metal-molecule contacts are an elusive yet important hurdle in the development of molecular electronic devices. This project explores the chemical synthesis of metal-molecule-metal structures for single-molecule spectroscopy and transport measurements. Conjugated thiol-azide molecules are self-assembled on gold nanoparticles, which are then linked with dialkyn bridge molecules using Sharpless “click” reactions.
12:15PM Q19.00006 Impact of Nanofillers on the Durability of Polymeric Coatings and Composites, LI-PIN SUNG, STEPHANIE WATSON, AARON FORSTER, Materials and Construction Research Division, National Institute of Standards and Technology; SHENG LIN-GIBSON, Polymer Division, National Institute of Standards and Technology — Metal oxide nanoparticles have been incorporated into polymer systems to improve durability performance properties, for example Ultra Violet (UV) degradation and scratch resistance. In this paper, we present recent research results on (1) the effect of particle dispersion and photoreactivity of TiO₂ on the UV degradation of polymeric coatings exposed to high intensity UV radiations at two different humidity conditions; (2) the impact of nano-SiO₂ concentration on surface mechanical properties (surface morphology and scratch behavior) of polymeric coatings and composites. The physical and chemical degradation of the coatings were monitored in periodic intervals using a combination of laser confocal scanning confocal microscopy (LSCM) and attenuated total reflectance-Fourier transform infrared spectroscopy. An instrumented nanoindentation and LSCM are utilized to measure surface modulus, perform scratch testing, and map scratch damage patterns. A strong impact on the durability performance in both studies was observed in the presence of nanofillers. Particularly in the scratch resistance study, the addition of nanofillers reduces surface roughness and increase scratch resistance of the nano-filler-polymer composites.

12:27PM Q19.00007 The “Music” of Silica-Poly(methyl methacrylate) Core-Shell Spheres: Eigenvibrations and Mechanical Properties at the Nanoscale, TIM STILL, Max Planck Institute for Polymer Research, Mainz, Germany (still@mpip-mainz.mpg.de), REBECCA SAINIDOU, Universite du Havre, Le Havre, France, GOETZ HELLMANN, Deutsches Kunststoffinstitut, Darmstadt, Germany, GEORGE FYTAS, MPI for Polymer Research, University of Crete and FORTH, Heraklion, Greece — We report on the measurement of elastic vibrational modes (eigenvibrations) in silica–poly(methyl methacrylate) (SiO₂–PMMA) core-shell spheres and corresponding spherical hollow capsules (PMMA) with different particle size (diameter: 232 nm–405 nm) and shell thickness (25 nm–112 nm) using Brillouin light scattering, supported by numerical calculations. [T. Still et al., Nano Lett. 8, 3194 (2008)] These localized modes allow to access the mechanical moduli of core and shell material. We observe redshifted eigenvibrations of silica–polymer core–shell spheres with a core thickness of 100 nm. Thereafter, we present the results obtained by using the model of a nanocomposite formed by the incorporation of the polyhedral oligomeric silsesquioxane (POSS) molecules in the crosslinked epoxy matrix. MD simulations were performed after the reaction mixture in the simulation box. The structures so generated are relaxed using a combination of molecular mechanics and molecular dynamics (MD) simulations. The approach utilizes simulated annealing optimization technique for carrying out one-step polymerization of the reaction mixture in the simulation box. The structures so generated are relaxed using a combination of molecular mechanics and molecular dynamics (MD) simulations. The developed technique is computationally efficient and has been used for creating atomistic model structures of both crosslinked epoxy and a nanocomposite formed by the incorporation of the polyhedral oligomeric silsesquioxane (POSS) molecules in the crosslinked epoxy matrix. MD simulations are used to determine the volume-temperature behavior of these structures. The hybrid hybrid model exhibits the desirable photolumincent properties of CdSe nanocrystals but does not fracture, as do thick electrochemically grown nanoparticle shells. The peculiar behavior of the vibrational modes in the hollow capsules is attributed to anisotropic dependence on overall size and layer thickness. The present investigation of the acoustical properties of the individual core-shell particles can lead to the use of such nanoscale engineered particles in more elaborate systems to control hypersonic phonons.

12:39PM Q19.00008 A Microscopic Model for the Reinforcement and the Non Linear Behaviour of Filled Elastomers and Thermoplastic Elastomers (Payne and Mullins Effects). DIDIER LONG, CNRS/Rhodia, SAMY MERABIA1, CNRS/Univ. Paris Sud, PAUL SOTTA, CNRS/Rhodia — We present a model regarding reinforcement properties of nano-structured polymers. Then, we show how it can be solved numerically by Dissipative Particles Dynamics. The model is based on the presence of glassy layers around the fillers. Strong reinforcement is obtained when these layers overlap. Key is the life-times distribution of these glassy bridges. The latter depend on polymer-filler interaction, the thermal–mechanical history, on the temperature, on the distance between fillers, and on the local stress in the material. Under applied strain, we show how the dynamics of yield and rebirth of glassy bridges account for the non-linear Payne and Mullins effects, which are a large drop of the elastic modulus at intermediate deformations, and a progressive recovery of the initial modulus when the samples are subsequently put at rest, respectively. These mechanisms account also for dissipative properties of filled elastomers. Our model opens the way for predicting mechanical behavior of nano-filled elastomers according to the filler structures and dispersion, polymer- filler interactions and temperature, in order to prepare systems with tailored properties.

12:51PM Q19.00009 Molecular Simulation of Highly Crosslinked Epoxy Resin and POSS-Epoxy Nanocomposites, PO-HAN LIN, RAJESH KHARE, Department of Chemical Engineering, Texas Tech University — Generation of atomistic model structures of crosslinked epoxy at realistic density is a challenging task. In this work, we present an efficient approach for generating such model structures with highly crosslinked matrices. The approach utilizes simulated annealing optimization technique for carrying out one-step polymerization of the reaction mixture in the simulation box. The structures so generated are relaxed using a combination of molecular mechanics and molecular dynamics (MD) simulations. The developed technique is computationally efficient and has been used for creating atomistic model structures of both crosslinked epoxy and a nanocomposite formed by the incorporation of the polyhedral oligomeric silsesquioxane (POSS) molecules in the crosslinked epoxy matrix. MD simulations were performed after the reaction mixture in the simulation box. The structures so generated are relaxed using a combination of molecular mechanics and molecular dynamics (MD) simulations. The hybrid model exhibits the desirable photolumincent properties of CdSe nanocrystals but does not fracture, as do thick electrochemically grown nanoparticle shells. The peculiar behavior of the vibrational modes in the hollow capsules is attributed to anisotropic dependence on overall size and layer thickness. The present investigation of the acoustical properties of the individual core-shell particles can lead to the use of such nanoscale engineered particles in more elaborate systems to control hypersonic phonons.

1:03PM Q19.00010 Reducing Strain in Electrophoretically Deposited Nanocrystal Films by Post-Deposition Incorporation of Polymers, THEODORE KRAMER, Department of Applied Physics and Applied Mathematics, Columbia University, STEFFEN JOCKUSCH, MICHAEL STEIGERWALD, NICHOLAS TURRO, Department of Chemistry, Columbia University, IRVING HERMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We have made dense nanoparticle-polymer films and investigated their mechanical properties using nano-indentation and other methods. Electrophoretically deposited (EPD) films of cadmium selenide nanocrystals were infiltrated with network-forming monomers and subsequently exposed to UV radiation in the presence of photoinitiators to facilitate polymerization of the monomer. This hybrid hybrid model exhibits the desirable photolumincent properties of CdSe nanocrystals but does not fracture, as do thick electrochemically grown nanoparticle shells. The peculiar behavior of the vibrational modes in the hollow capsules is attributed to anisotropic dependence on overall size and layer thickness. The present investigation of the acoustical properties of the individual core-shell particles can lead to the use of such nanoscale engineered particles in more elaborate systems to control hypersonic phonons.

1:15PM Q19.00011 Mechanics of Nanoscale composite films from stress-electrical measurements: A nanoscale foam, CHIEU NGUYEN, VIVEK MAHESHWARI, RAVI SARAF, CHEMICAL ENGINEERING-UNIVERSITY OF NEBRASKA-LINCOLN TEAM — Nanometer thin (> 100nm) composite films consisting of polymers and organic-inorganic materials such as nanoparticles, quantum dots, nanotubes and dyes are widely researched for applications in designing a bio-mimetic cell membrane, solar cells, electronic and optical sensors, ion separation membranes and coatings. Being nanoscale in dimensions the mechanical properties of the film is critically governed by its morphology at nanoscale and the mutual interaction between the constituents of the film. The assembly process and the components of the film are detrimental in defining its morphology. A vast array of film morphologies is possible due to the multitude of combinations in processing and the components available to make the film. Sensors, ion separation membranes and coatings. Being nanoscale in dimensions the mechanical properties of the film is critically governed by its morphology at nanoscale and the mutual interaction between the constituents of the film. The assembly process and the components of the film are detrimental in defining its morphology. The study of mechanical properties of the film is hence important due their application in multitude of fields and correlating it to the nanoscale morphology and properties of its constituents. Here we present the stress-electrical measurements on a nanoscale (~100nm) nanocomposite film prepared using the well known spin assisted ionic self-assembly process. The film is a stack of nanoparticle layers, spaced by dielectric layer. Each dielectric layer consists of a stack of alternating anionic and cationic polyelectrolyte layers. The separation between the nanoparticle layers can be controlled with nanometer scale precision by modulating the number of polyelectrolyte layers in each dielectric layer.
1:27PM Q19.00012 Local dielectric permittivity profiles of sapphire/polypolypropylene interfaces, LIPING YU, V. RANJAN, M. BUONGIORNO NARDELLI, J. BERNHOLC, NC State U — Recently, the need for high-power-density capacitors has stimulated research to develop composite dielectric materials with high-k nanoparticles embedded in a polymer matrix. In these materials, surfaces and interfaces may play an important role in determining the overall dielectric properties. We present first-principles investigations of the dielectric permittivity profiles across slabs and interfaces of sapphire($\alpha$-Al$_2$O$_3$)/isotactic-polypropylene(IPP). Our results indicate that the permittivity profile at interface strongly depends on the nanoscale averaging procedure. We propose an averaging model that ensures near-locality of the dielectric function. We find that: (i) the dielectric permittivity approaches the corresponding bulk value just a few atomic layers away from the interface or surface; (ii) the dielectric constant is enhanced at the surfaces of the isolated $\alpha$-Al$_2$O$_3$ slabs, while no enhancement is observed at the IPP slab surfaces; and (iii) the dielectric transition at the $\alpha$Al$_2$O$_3$/IPP is mainly confined in the $\alpha$Al$_2$O$_3$ side.

1:39PM Q19.00013 Flow induced orientation behavior of concentrated dispersions of multi-wall carbon nanotube suspensions under shear flow: Effect of aspect ratio and concentration, SASWATI PUJARI, WESLEY BURGHARDT, University of Massachusetts-Amherst, SAMEER RAHATEKAR, JEFFREY GILMAN, National Institute of Standards and Technology, KRZYSZTOF KOZIOL, ALAN WINDLE, Cambridge University — We report studies of average orientation state of concentrated dispersions of multi-walled carbon nanotube (MWNTs) in steady shear flow. Uncured epoxy was used as a viscous, Newtonian suspending medium, and samples were prepared from ‘aligned’ MWNTs using methods previously reported (Rahatekar et al., J Rheol 40:599, 2006). Flow induced structural measurements were made in the vorticity (1-3) plane of simple shear flow using in-situ wide angle x-ray scattering techniques in a rotating disc shear cell. Azimuthally-dependent diffraction from the internal layered structure of the MWNTs was used to characterize alignment. Steady state anisotropy of MWNT dispersions decrease with increasing the length of the MWNTs. Surprisingly, the anisotropy is seen to increase with increasing concentration. For one of the samples, more detailed orientation dynamics are studied in steady shear and transient shear flow both in the 1-2 (flow gradient) and 1-3 (vorticity) planes of shear flow, and through comparison of wide-angle and small-angle scattering signatures of flow-induced nanotube alignment.

1:51PM Q19.00014 Polymorphism in electrospun poly(vinylidene fluoride)/nanoclay composite nanofibers, LEI YU, PEGGY CEBE, Tufts University — We investigated the morphology and polymorphism behavior of electrospun (ES) composite nanofibers of poly(vinylidene fluoride) (PVDF) with two nanoclays: Lucentite$^{TM}$ STN and SWN. Lucentite$^{TM}$ STN and SWN synthetic nanoclays are based on hectrite structure, but only STN contains an organic modifier between the hectrite layers. The PVDF was dissolved, and nanoclay was dispersed, in N,N-dimethylformamide/acetone and then electrospun into nanofibers with diameters ranging from 100∼1000 nm. The nano-assembly content ranged from 0.2% to 10%. The addition of STN can greatly decrease the number of beads and makes the diameter of the ES nanofibers more uniform due to an increase of solution conductivity. From wide angle X-ray scattering and Fourier transform infrared spectroscopy, we found both STN and SWN can induce more beta phase PVDF.

2:03PM Q19.00015 Polymer/inorganic nanocomposites with prescribed morphologies, E. MANIAS, M.J. HEIDECCKER, J. ZHANG, G. POLIZOS, Materials Sci & Eng, Penn State U — Despite the proliferation of polymer/inorganic nanocomposites in academic research and the commercialization of tens of products based on such materials, their true potential still remains largely untapped. One of the major hurdles in this endeavor is to capitalize on the novel properties afforded by a true--nanophase morphology. Since these are beyond simple nanoparticulate dispersions and towards prescribed filler/phase arrangements and tailored filler--polymer interfaces. We comparatively present nanocomposites with prescribed nanostructures, which can be made in large, industrial-scale, quantities (e.g. composites with spatially arranged fillers: such as shear-aligned fillers in blown PE films and filler-induced compatibilization of PC/PET blends). We discuss the fundamental mechanisms of achieving the prescribed nanostructures and the related novel functionalities. In particular, we emphasize on extraordinary properties achieved by simultaneous control of the composite morphology and of the polymer--filler interface, such as an impressive toughening effect in PC/PET nanocomposites, and PE nanocomposites with a predetermined tensile strength by tailoring the polymer--filler interfacial adhesion.

Papers in session Q19.00012-015 have been collected and published as a special issue of Polymer in the Journal of Energy Storage. The issue is available for purchase from the American Chemical Society.

Wednesday, March 18, 2009 11:15AM - 2:15PM –
Session Q20 DPOLY: Thin Films and Adhesion I

11:15AM Q20.00001 Capillary wrinkling of a floating sheet under differential surface tension, JIANGSHUI HUANG, Department of Physics & Department of Polymer Science and Engineering, University of Massachusetts-Amherst, WIM H. DE JEU, Department of Polymer Science and Engineering, University of Massachusetts-Amherst, NARAYANAN MENON, Department of Physics, University of Massachusetts-Amherst, THOMAS P. RUSSELL, Department of Polymer Science and Engineering, University of Massachusetts-Amherst — We have previously studied the wrinkling of a thin polymer film floating on the surface of water under the capillary force exerted by a drop of water placed on its surface. Here, the same surface tension both sets the radial stress in the unperturbed film as well as the source of the perturbation that leads to the wrinkling instability. We now report the effect on the wrinkling instability of a differential surface tension by using fluids with different surface tensions for the liquid the film is floating on and the drop put on the film. We use both surfactants and a variety of pure liquids to control the surface tension of water. When the base radial stress of the filmed floating was decreased, the length of the wrinkles increased, but the number of wrinkles decreased.


11:27AM Q20.00002 Effect of Long-chain Branching on Surface Dynamics of Polymer Films, MARK D. FOSTER, SHIH-FAN WANG, JAE SIK LEE, SÉWÔO YANG, Dept. of Polymer Science, The University of Akron, ZHANG JIANG, SURESH NARAYANAN, X-ray Science Division, Argonne National Lab, DAVID WU, Colorado School of Mines — Thermally stimulated fluctuations of the surface of films of branched polystyrene chains have been studied using x-ray photon correlation spectroscopy (XPCS), a recently-developed technique that has already been applied to study the surfaces of melts of linear polystyrene chains. Surface relaxations of films of branched chains are faster than are those of films of linear analogs. However, the Tg’s of the branched molecules are also lower. The variation in surface relaxation time as a function of scattering vector can be described well by a continuum hydrodynamic theory of thermally stimulated capillary waves with a no-slip boundary condition. However, the film viscosities inferred from fits of the theory to the data differ markedly from viscosities from bulk measurements. Acknowledgements: NSF support (CBET 0730692)
12:03PM Q20.00005 Dimension-Dependent Mechanical Properties of Pure and Antiplasticized Polymer Nanostructures, SEAN DELCAMBRE, ROBERT RIGGLEMAN, JUAN DE PABLO, PAUL NEALEY, Department of Chemical and Biological Engineering, University of Wisconsin - Madison — Dense arrays of poly(methyl methacrylate) (PMMA) grating nanostructures 80 nm to 120 nm in pitch were fabricated by electron-beam and extreme ultraviolet interferometric lithography. During development and rinse drying, the nanostructures are subjected to capillary forces that are defined by the rinse fluid properties and spacing between adjacent structures. The applied capillary forces and structure aspect ratios were varied experimentally to induce structure collapse. By coupling nanostructure collapse data with continuum cantilever beam bending models, mechanical properties such as the elastic modulus and yield stress are determined. The elastic moduli of PMMA structures at this scale are observed to decrease with structure width. This behavior is counteracted by the addition of a low molecular weight diluent, tris(2-chloropropyl) phosphate (TCPP). At concentrations up to 5 wt%, TCPP acts as an antiplasticizing agent, decreasing the glass transition temperature while simultaneously increasing the elastic modulus. For a given applied capillary force, nanostructures containing 5 wt% TCPP are observed to remain stable at aspect ratios up to 20% higher than the pure material.

12:15PM Q20.00006 The stiffening of ultrathin polymer films in the rubbery regime – the relative contributions of bending, membrane stress and surface tension, PAUL O’CONNELL, GREGORY MCKENNA, Texas Tech University — A novel nano-bubble inflation technique has been developed which allows the determination of the absolute creep compliance of ultrathin polymer films as thin as 9 nm. Previous results have shown that the degree of reduction in Tg with film thickness is not universal, with PVAc showing no change in Tg down to 23nm while PS shows a significant reduction at thicknesses below approximately 80nm. Interestingly the rubbery compliance of ultrathin polymer films as thin as 9 nm. Previous results have shown that the degree of reduction in Tg with film thickness is not universal, with PVAc showing no change in Tg down to 23nm while PS shows a significant reduction at thicknesses below approximately 80nm. Interestingly the rubbery

12:27PM Q20.00007 Molecular confinement and residual stress in ultrathin polymer films, ARNOLD YANG, National Tsing Hua University, GUNTER REITER, University of Freiburg, Germany, YI-HSIN CHANG, YI CHIEN, National Tsing Hua University — The residual stress operative in thin films of a polymer (polystyrene) prepared by spin coating was determined from local elastic stress release induced by pinhole nucleation during dewetting instability. The measured stress was orders of magnitude greater than the capillary force and attributed to chain recoiling of the confined macromolecules. The entropy-driven stress was found to be small for thicker films but increase dramatically as film thickness became less than the unperturbed molecular dimensions. The chain conformations in these films can only be described by the Langevin, rather than Gaussian, statistic and the draw ratio was determined to be around 5, comparable to that in craze fibrils, for film thickness of 4 nm. The effects of spin speed, aging-induced relaxation, and molecular packing were investigated. The molecular processes during spin coating were proposed. In addition, conjugated polymers when squeezed into the molecular thicknesses were found to emit light with much enhanced efficiencies due to the large molecular deformation.

12:39PM Q20.00008 Semifluorinated Polymers Confined at the Solid-Air Interface, UMESH SHRESTHA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHA, Clemson University — Effective responsive layers should exhibit stability while retaining a dynamic mode that will allow reaction of the interface to external stimuli. Semifluorinated polymers have a potential for forming energy controlled responsive interfaces. Because of the high segregation between the fluorinated and protonated segments, well defined structures are induced at relatively short chains, retaining the capability to rearrange on short time scales. Fluorinated segments affect the interfacial energies as well as enhance thermal stability and controls the refractive index and dielectric properties. The present study investigates the interfacial response of poly trifluoro propylmethyl siloxane-polystyrene diblock copolymer (PTFPMPS-PS) at volume fractions varying from 0.003 to 0.5 of fluorinated block, at the interface of oxidized silicon wafers. In all volume fractions we found that the air interface is fluorine rich and the solid surface in proton rich. Layering is detected across the films for all volume fractions. Upon annealing the layering is retained, however the interfacial compositions change.
Spatially Organized Polymer Films Prepared by Oblique Angle Polymerization.


This work was supported National Science Foundation.
11:15AM Q21.00001 High-Resolution Spectroscopy with a Free-Electron Laser: Vibrational Lifetimes of Hydrogen-related Defects in Silicon1,2, GUNTER LUEPKKE, College of William and Mary — Gunter Luempke, Department of Applied Science, The College of William and Mary, Williamsburg, VA 23187 Vibrational lifetimes of hydrogen- and deuterium-related bonding and stretching modes in crystalline silicon are measured by high-resolution infrared absorption spectroscopy and pump-probe transient bleaching technique using the Jefferson Lab. Free-Electron Laser. We find that the vibrational lifetimes of the bending modes follow a universal frequency-gap law, i.e., the decay time increases exponentially with increasing decay order, with values ranging from 1 ps for a one-phonon process to 265 ps for a four-phonon process. The temperature dependence of the lifetimes shows that the bending mode decays by lowest-order multi-phonon process. In contrast, the lifetimes of the stretching modes are found to be extremely dependent on the defect structure, ranging from 2 to 295 ps. Against conventional wisdom, we find that lifetimes of Si-D stretch modes typically are longer than for the corresponding Si-H modes. Our results provide new insights into vibrational decay and the giant isotope effect of hydrogen in semiconductor systems. The potential implications of the results on the physics of electronic device degradation are discussed.

1We thank the National Science Foundation and the Department of Energy for their financial support.

11:51AM Q21.00002 First-Principles Calculation of Carrier Lifetimes in Semiconductors1,2, VINCENZO LORDI, PAUL ERHART, DANIEL ABERG, Lawrence Livermore National Lab, Livermore, CA — We have developed first-principles methods based on density functional theory to calculate carrier lifetimes in semiconductors related to trapping on deep-level defects. Lifetimes are determined based on Schottky–Read–Hall theory, using recombination rates calculated from first principles for several competing mechanisms: radiative recombination, phonon-assisted (nonradiative) recombination, and Auger recombination. The recombination rates are calculated within a fully first-principles framework with no empirical parameters. We have recently applied these methods to study the role of native and impurity defects in reducing carrier lifetimes in bulk single-crystal aluminum antimonide (AlSb) and cadmium telluride (CdTe), two promising materials for high-resolution room-temperature gamma radiation detection.

1Prepared by LLNL under Contract DE-AC52-07NA27344

12:03PM Q21.00003 Fully ab initio supercell corrections for charged defects, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max-Planck-Institut for Iron Research, Duesseldorf, Germany, CHRIS G. VAN DE WALLE, Materials Department, University of California Santa Barbara — Charged point defects govern the carrier densities in semiconductors and are crucial for the performance of electronic devices. However, quantifying the thermodynamical, chemical, and electrical properties of such defects is a challenge to both experiment and theory. In ab-initio calculations, the defect is usually modeled in a periodic supercell with a few dozen to a few hundred atoms. Unfortunately, this introduces artificial electrostatic interactions between charged defects. A number of correction schemes such as Makov-Payne corrections, potential alignment, scaling laws, or Coulomb truncation, are available in the literature, but they often fail to remove the supercell dependence completely. The assumptions behind these schemes are sometimes unclear and all schemes lack a stringent theoretical foundation. From a formal analysis within linear-response theory, we propose a new and simple scheme that combines the strengths of Makov-Payne corrections and potential alignment. Our scheme requires no empirical parameters or fitting procedures. Its reliability is demonstrated even in extreme cases.

12:15PM Q21.00004 Optimal Silicon for Photovoltaic Applications, GEORGY SAMSONIDZE, MARVIN L. COHEN, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 — A small overlap of the silicon optical absorption spectrum with the solar emission spectrum limits the efficiency of silicon-based solar cells. We conduct a theoretical search for substitutionally doped silicon with the aim to maximize the spectral overlap. Different dopant species at various concentrations compatible with the existing silicon technology are examined in the virtual crystal approximation using the empirical pseudopotential method. The optimal doping configurations found are further investigated with a first-principles many-electron Green’s function approach. The optical absorption spectrum of the doped silicon is calculated by solving the Bethe-Salpeter equation which includes excitonic effects. This work was supported by National Science Foundation Grant No. DMR07-05941, and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NSF through TeraGrid resources at Indiana University and TACC.

12:27PM Q21.00005 Microprobe X-ray Absorption Spectroscopy of Chalcogen Doped Silicon, BONNA NEWMAN, JOE SULLIVAN, Massachusetts Institute of Technology, MARK WINKLER, MENG-JU SHER, Harvard University, MATTHEW MARCUS, Advanced Light Source, Lawrence Berkeley National Lab, MATTHEW SMITH, SILVIJA GRADEC, Massachusetts Institute of Technology, ERIC MAZUR, Harvard University, TONIO BUNASSISI, Massachusetts Institute of Technology — Doping Si with chalcogen atoms (S, Se, and Te) in excess of the solubility limit has been shown to result in optical absorption below the bandgap. This material, known as “black silicon”, is promising for infrared photon detectors and possibly photovoltaic devices. We report on the relationship between the chemical state of the dopant atoms and infrared absorption properties. A high concentration of 10^20 dopant atoms/cm^3 in the near-surface layer allows for extended X-ray absorption fine structure (EXAFS) investigations and determination of chemical state. We combine these results with absorption measurements and Auger spectroscopy to understand the correlations between optical and structural properties of chalcogen doped Si.

12:39PM Q21.00006 Hydrogen in multi-crystalline Si used for the fabrication of solar cells1,2, CHAO PENG, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University, LODI CARNEL, REC Scanwafer AS — The multicrystalline Si materials that are used by industry to fabricate solar cells often contain a high concentration of carbon impurities. Furthermore, hydrogen is also commonly introduced during processing to improve solar-cell performance.1,2 At present, the H- and C-related defect reactions that occur and what their effect might be remain poorly understood. We have performed a series of experiments in which IR spectroscopy has been used to study a family of defect complexes that are formed when H is trapped by substitutional carbon impurities in multi-crystalline Si. The structures, concentrations, and thermal stabilities of these defects have been investigated.


1Supported by NSF grant DMR 0802278 and the Silicon Solar Consortium.

12:51PM Q21.00007 Effect of copassivation of Cl and Cu on CdTe grain boundaries, LINXIN ZHANG, JUAREZ L.F. DA SILVA, National Renewable Energy Laboratory, JINGBO LI, Institute of Semiconductors, CAS, Beijing, China, YANFA YAN, T.A. GESSERT, SU-HUAI WEI, National Renewable Energy Laboratory — Grain boundaries (GBs) and dislocations are generally viewed as detrimental to device applications, because they usually contain a high density of deep defect levels that act as recombination centers for charge carriers. Surprisingly, two leading polycrystalline thin-film solar cells based on CuInSe2 (CIS) and CdTe have produced very high efficiencies of 20% and 16.5%, respectively, despite that these materials contain significant amounts of GBs. Using a first-principles method, we investigate the structural and electronic properties of GBs in polycrystalline CdTe and the effects of copassivation of elements with far distinct electronegativities. Of the two types of GBs studied in this work, we find that the Cd core is less harmful to the carrier transport, but is difficult to passivate with impurities such as Cl and Cu, whereas the Te core creates a high defect density below the conduction band minimum, but all these levels can be removed by copassivation of Cl and Cu. Our analysis indicates that for most polycrystalline systems copassivation or multipassivation is required to passivate the GBs.
1:03PM Q21.00008 Influence of Crystalline Defects in GaN-InGaN Solar Cells, BALAKRISHNAM JAMPANA, NIKOLAI FALEV, University of Delaware, IAN FERGUSON, Georgia Tech, ROBERT OPILA, University of Delaware, CHRISTIANA HONSBERG, Arizona State University — Crystalline defects originating from lattice-mismatch in epitaxial materials appear to be the dominant factor reducing high efficiency solar cell performance. In this paper we present an explanation of the observed structural and optical characteristics originating in lattice-mismatched III-nitride epilayer materials. This model is based on creation, diffusion, accumulation and structural transformation of point defects to extended crystalline defects. In this work InGaN photovoltaic structures are grown by MOCVD on GaN templates with thicknesses in the 50 to 400nm range. The types and spatial distribution of crystalline defects are determined from XRD rocking curves and reciprocal space maps. The crystalline quality is observed to deteriorate with increasing thickness and growth rate. Wide band gap InGaN based solar cells require 150 to 400nm of active layer thicknesses and crystalline defects are observed in this thickness range degrading the solar cell performance. A physical model correlating the response of the solar cell to the type and spatial distribution of the defects will be presented. The work will aid improve the crystalline quality of InGaN for application as high efficiency solar cells.

1:15PM Q21.00009 Scanning Probe Spectroscopy of Individual Dopants in Silicon, MOREWELL GASSELLER, MATTY CAMAX, ROGER LOO, SVEN ROGGE, STUART TESSMER — A key goal of semiconductor electronics is to develop devices based on manipulation of the charge and spin of individual dopant atoms. Elucidating the quantum structure of these minute systems is a difficult technical challenge. Here we present capacitance-based scanned-probe measurements that both spatially-resolve individual subsurface boron dopants in silicon and detect spectroscopically single holes entering the Bi + state of these atoms. We observe that, on average, acceptors with a closer nearest neighbor exhibit stronger binding. This finding is consistent with the interpretation of resonant tunneling measurements performed on a similar sample.

1:27PM Q22.00010 Vacancy-related defects and the E'Δ center in amorphous silicon dioxide, BLAIR TUTTLE, Penn State Erie, SOKRATES PANTELIDES, Vanderbilt University — The microscopic identification of vacancy-related defects in silicon dioxide has been a major challenge. Particularly in amorphous silica, the role of vacancy clusters is still controversial. Experimental data have led to suggestions that the E' center might be a four-vacancy cluster instead of a single vacancy. Here we report density functional calculations of single vacancies and clusters of four vacancies in realistic models of amorphous silica. Results for single vacancies compare well to previous theory. A key result for four-vacancy clusters is that relaxations localize the unpaired electron preferentially on one Si atom, resulting in a strongly anisotropic electron-paramagnetic-resonance signal. Atoms in single vacancies have a more benign anisotropy which is more compatible with the observed isotropic signal. This work was supported by the Air Force Office of Scientific Research under a MURI grant (FA9550-05-1-0306) and by the US Navy.

1:39PM Q21.00011 Enhanced defect generation in gate oxides of p-channel MOS transistors in a moisture ambient, ARITRA DASGUPTA, S.A. FRANCIS, D.M. FLEETWOOD, Department of Electrical Engineering and Computer Science, Vanderbilt University — Transistors and ICs built in Sandia’s 4/3 μm technology were exposed to moisture, irradiated, and annealed. The moisture exposures were performed using highly accelerated stress test (HAST) at 130°C and 85% relative humidity. Irradiation of n-channel transistors exposed to HAST followed by a long-term anneal resulted in some increase in interface-trap and oxide-trapped charge buildup. We observed enhanced post-irradiation defect generation of oxide trapped charge, interface traps and border traps in the gate oxides of p-channel MOS transistors that were exposed to humidity. This is characterized by enhanced voltage shifts due to oxide trapped charge and interface traps observed in the p-channel transistors. Low frequency noise measurements also showed enhanced low frequency noise power in moisture exposed p-channel transistors. Our results indicate that there are enhanced precursor hole trap defects or oxygen vacancies present in the gate oxide of p-channel transistors as a result of presence of moisture or hydrogen ambient. The smaller voltage shifts in the n-channel transistors may be related to the presence of phosphorus atoms in the gate oxides.

1:51PM Q21.00012 Carbon clusters as possible defects at the SiC-SiO2 interface, YINGDI LIU, HONGLI DANG, YANG LIU, YING LI, University of Tulsa, MATTHEW CHISHOLM, Oak Ridge National Laboratory, TRINITY BIGGERSTAFF, North Carolina State University, GERD DUSCHER, University of Tennessee, Knoxville, SANWU WANG, University of Tulsa — High state densities in the band gap of the SiC-SiO2 interface significantly reduce the channel mobilities in SiC-based high-temperature/high-power microelectronics. Investigations of the nature of the interface defects are thus of great importance. While several possible defects including very small carbon clusters with up to four carbon atoms have been identified as first-principal theory, larger carbon clusters as possible defects have attracted less attention. Here, we report first-principles quantum-mechanical calculations for two larger carbon clusters, the C12 ring and the C20 fullerene, on the SiC-SiO2 interface. We find that both carbon clusters introduce significant states in the band gap. The states extend over the entire band gap with higher densities in the upper half of the gap, thus accounting for some of the interface trap densities observed experimentally.

2:03PM Q21.00013 First-principles study of local (p×2×2) structures on Si(100) surface, MIN-KOOK KIM, HYOONG JUON CHOI, Department of Physics and IPAP, Yonsei University — We study structural defects inducing local (p×2×2) structures in c(4\times8)-reconstructed Si(100) surface, using an ab-initio pseudopotential density functional method. The local density approximation to the density functional theory is used and electronic wavefunctions are expanded with pseudo-atomic orbitals. The atomic structures of defects are optimized by minimizing the total energy. Our calculations show that the defects increase the total energy of the system but they are energetically stable with energy barrier. STM images for occupied and unoccupied states are simulated to investigate the surface electronic structures. Effects of electron doping and external electric field on the defects are also studied. This work was supported by the KRF (KRF-2007-314-C00075) and by the KOSEF Grant No. R01-2007-000- 20922-0. Computational resources have been provided by KISTI Supercomputing Center (KSC-2008-S02-0004).

Wednesday, March 18, 2009 11:15AM - 2:15PM –
Session Q22 GMAG DMP FIAP:
Focus Session: Spins in Quantum Dots and Mn in Arsenides

11:15AM Q22.00001 Intershell Exchange and Sequential Electrically Injected Spin Populations of InAs Quantum-Dot Shell States, GEORGE KIOSEOGLOU, Naval Research Laboratory and University of Crete — Quantum dots (QDs) are attractive for a variety of spintronic applications. Their electronic structure exhibits the s, p, d, f shells characteristic of atoms. We report electrical injection of spin-polarized electrons from Fe contacts into the individual shells of highly uniform self-assembled InAs QDs, and we determine the s-p and p-d intershell exchange using circular polarization of the electroluminescence (EL) spectra. This work was supported by the NSF (CMS-0645953), by the Oak Ridge Associated Universities, by the National Center for Supercomputing Applications (TG-DMRO080005N), and by the National Center for Computational Sciences at Oak Ridge National Laboratory.

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11:15AM Q22.00001 Intershell Exchange and Sequential Electrically Injected Spin Populations of InAs Quantum-Dot Shell States, GEORGE KIOSEOGLOU, Naval Research Laboratory and University of Crete — Quantum dots (QDs) are attractive for a variety of spintronic applications. Their electronic structure exhibits the s, p, d, f shells characteristic of atoms. We report electrical injection of spin-polarized electrons from Fe contacts into the individual shells of highly uniform self-assembled InAs QDs, and we determine the s-p and p-d intershell exchange using circular polarization of the electroluminescence (EL) spectra. This work was supported by the NSF (CMS-0645953), by the Oak Ridge Associated Universities, by the National Center for Supercomputing Applications (TG-DMRO080005N), and by the National Center for Computational Sciences at Oak Ridge National Laboratory.

12:03PM Q22.00003 Mn doping of InAs quantum dots studied by X-STM. , PAUL KOENRAAD, MURAT BOZKURT, JENS GARLEFF, Eindhoven University of Technology, VICKY GRANT, RICHARD CAMPION, TOM FOXON, University of Nottingham, EUCLYDES MAREGA, University of San Carlos, GREG SOLOMON, University of Arkansas — We report on the X-STM analysis of Mn doped quantum dots. The X-STM technique allows one to tune the temperature with a given temporal contrast to build an image of the spin thermopower coefficient in a junction as large as the Seebeck coefficient, resulting in a large spin figure of merit. In addition, it demonstrates that the junction can be tuned to supply only spin current but no charge current. We also discuss experimental systems where our predictions can be verified.

1This work is supported by the DOE.

12:15PM Q22.00004 Thermo-spin effects in quantum dots connected to ferromagnetic leads

YONATAN DUBI, MASSIMILIANO DI VENTRA, University of California - San Diego — We study a system composed of a quantum dot in contact with ferromagnetic leads held at different temperatures, which we suggest can be used as a source of spin-voltage. Spin analogs to the thermoelectric and thermoelectric figure of merit of metallic systems are studied, and we show how to make a more precise measurement of the spin thermopower coefficient in a junction as large as the Seebeck coefficient, resulting in a large spin figure of merit. In addition, it demonstrates that the junction can be tuned to supply only spin current but no charge current. We also discuss experimental systems where our predictions can be verified.

12:27PM Q22.00005 Tunnel magnetoresistance in mesoscale (Ga,Mn)As magnetic tunnel junctions. , PARTHA MITRA, MARK J. WILSON, MENG ZHU, PETER SCHIFFER, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802, KIRAN V. THADANI, DAN C. RALPH, Dept. of Physics, Cornell University, Ithaca NY 14853 — We recently demonstrated exchange-biased magnetic tunnel junctions (MTJs) built from the ferromagnetic semiconductor (Ga,Mn)As [Phys. Rev. B. 78, 195307 (2008)]. Here, we report measurements of the tunnel magnetoresistance (TMR) in mesoscale (Ga,Mn)As MTJ devices with areas that range from ~1 to 100 μm², mapping out the TMR as a function of the magnetic field vector and the sample temperature. The vector field measurements provide insights into the interplay between the magnetic anisotropies of (Ga,Mn)As. In contrast to our earlier studies large area devices, we find that the TMR in these mesoscale devices increases exponentially with decreasing temperature, with a form exp(-T/T*). At temperatures lower than T*, the conductance-voltage characteristics show a strong dependence, suggesting the role of Coulomb interactions in the spin-dependent tunneling process in these small area MTJs. Work supported by the ONR MURI program.

12:39PM Q22.00006 Spectra broadening in Point-Contact Andreev Reflection Measurement on GaMnAs , SHANG-FAN LEE, T.W. CHIANG, Y.H. CHIU, S.Y. HUANG, Institute of Physics, Academia Sinica, Taipei, Taiwan, Republic of China, J.J. LIANG, Department of Physics, Fu Jen Catholic University, Taipei, Taiwan, Republic of China, H. JAFFRES, J.M. GEORGE, Unite Mixte de Physique CNRS/Thales and Universite Paris-Sud, Orsay, France, A. LEMAITRE, Laboratoire de Photonique et de Nanostructure, CNRS, Marcoussis, France — Point-Contact Andreev Reflection (PCAR) technique has been considered as a reliable method for determining electron spin polarization of novel metallic ferromagnets. For dilute magnetic semiconductors, this is less applicable due to the resistive nature of the material. We investigate PCAR spectra of GaAs/MnAs systems using Pb tips. The observed spectrum exhibits behaviors described in the Modified Blonder-Tinkham-Klapwijk (MBTK) model but with a significant spectrum broadening. Modified BTK theory is commonly applied to analyze PCAR spectra with electron polarization, superconducting energy gap, and interface transparency as parameters. We present an analysis based on the introduction of spreading resistance and the inelastic scattering at the interface. In as-grown and annealed samples, we extract spin polarization of 76%/74% from our analysis, both smaller than the value obtained from approach of effective temperature, 90%/82%.

12:51PM Q22.00007 Ultrafast Photoinduced Coherent Spin Dynamics in Ferromagnetic Ga₀.₉₋ₓMnₓAs/GaAs Structure

JINGBO QI, YING XU, ANDREW STEIGERWALD, NORMAN TOLK, Vanderbilt University, XINYU LIU, JACEK FURDYNA, University of Notre Dame, ILIAS PERAKIS, University of Crete — Ultrafast pump-probe magneto-optical spectroscopy is used to study coherent spin dynamics in the ferromagnetic semiconductor Ga₀.₉₋ₓMnₓAs systems. Above GaAs bandgap E_g, the temporal Kerr signal is found to be strongly dependent on pump photon polarization. This polarization dependence is attributed to spins of electrons photoexcited to the conduction band, and disappears for E_p< E_g. Below the Curie temperature T_C of the Ga₀.₉₋ₓMnₓAs samples, the temporal Kerr rotation acquires an additional oscillatory component, attributed to the precession of the ferromagnetically-coupled Mn spins. This precession is observed for excitation above and below E_g, regardless of the pump polarization states. The detailed characteristics of this ferromagnetic precession are discussed in terms of the Landau-Lifshitz-Gilbert (LLG) model.

3This work was supported by DOE through Grant DE-FG02-99ER45781 (Vanderbilt), NSF under Grant DMR06-03752 (Notre Dame), and by EU STREP program HYSWITCH (Crete).

1:03PM Q22.00008 Temperature Dependence of Anomalous Hall Effect in Metallic (Ga,Mn)As films

XINYU LIU, ZHIQI GE, SHAOPING SHEN, MARGARET DOBROWOLSKA, JACEK FURDYNA, Department of Physics, University of Notre Dame, Notre Dame, IN 46556 — We present a systematic study of the temperature dependence of anomalous Hall effect (AHE) in metallic (Ga,Mn)As films. The Hall effect in (Ga,Mn)As is described as ρ_yx = R_0 + cρ_x M_x, where R_0 (1/μ) is the ordinary Hall coefficient, ρ_x and ρ_y are the transverse and longitudinal resistivities, and c is a scaling parameter. In this work we have developed a self-consistent method to determine R_0, c and n simultaneously. We use this method to analyze the Hall and resistivity data measured up to B = 6 T at various temperatures. We find that for the metallic samples, a distinct evolution of the AHE occurs as temperature increases, as evidenced by the temperature dependence of the parameter c. We propose that the correlation between the AHE and the resistivity should be reconsidered by using a two-component model in order to separate contributions due to different scattering mechanisms.
Antiferromagnetic interlayer exchange coupling in Ga$_{1-x}$Mn$_x$As/GaAs diluted ferromagnetic semiconductor multilayers. JAE-HO CHUNG, S.J. CHUNG, SANGHOON LEE, Korea University, B.J. KIRBY, J.A. BORCHERS, NIST Center for Neutron Research, Y.J. CHO, X. LIU, J.K. FURDYNA, University of Notre Dame — We use neutron reflectometry to investigate the interlayer exchange coupling between Ga$_{0.97}$Mn$_{0.03}$As ferromagnetic semiconductor layers separated by non-magnetic Be-doped GaAs spacers. Polarized neutron reflectivity measured below the Curie temperature of Ga$_{0.97}$Mn$_{0.03}$As reveals a characteristic splitting at the wave vector corresponding to twice the multilayer period, indicating that the coupling between the ferromagnetic layers is antiferromagnetic (AFM). When the applied field is increased to above the saturation field, this AFM coupling is suppressed. This behavior is not observed when the spacers are undoped, suggesting that the observed AFM coupling is mediated by charge carriers introduced via Be doping. The behavior of magnetization of the multilayers measured by DC magnetometry is consistent with the neutron reflectometry results.

Engineering the interlayer exchange coupling in hybrid ferromagnetic metal/semiconductor heterostructures. MARK J. WILSON, MENG ZHU, PETER SCHIFFER, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802, ROBERTO C. MYERS, DAVID D. AWSCHALOM, Dept. of Physics, University of California, Santa Barbara, CA 93106, MICHAEL E. FLATTE, Dept. of Physics, University of Iowa, Iowa City, IA 52242 — The systematic study of the exchange coupling in ferromagnetic semiconductor heterostructures is important for developing proof-of-concept spin transfer semiconductor devices. We recently demonstrated interlayer exchange coupling between a ferromagnetic semiconductor (Ga$_{1-x}$Mn$_x$As) and a ferromagnetic metal (MnAs) [APL 91, 192503 (2007)]. Here, we report a comprehensive magnetochemistry study of the underlying exchange coupling in this hybrid system. We vary key parameters such as the thicknesses of both the ferromagnetic layers and the composition of the Ga$_{1-x}$Mn$_x$As layer, and examine our observations using an “exchange spring” model. We also demonstrate the propagation of the exchange coupling through a non-magnetic spacer layer (p-doped GaAs) and examine the variation of this coupling as a function of the spacer layer thickness and doping. Work supported by the ONR MURI program and by NSF.

Solubility control in dilute magnetic semiconductors by using the co-doping method. KAZUNORI SATO, HITOSHI FUJII, ISIR, Osaka University, LARS BERGGVIST, PETER H. DEDERICHS, IFF, FZ-Juelich, HIROSHI KATAYAMA-YOSHIDA, Osaka University — To overcome low solubility limit of magnetic impurities in dilute magnetic semiconductors (DMS) and realize room temperature ferromagnetism, we propose a co-doping method to increase solubility of magnetic impurities in DMS [1]. We calculate electronic structure of (Ga, Mn)As, (Ga, Mn)N, (Ga, Cr)N and (Zn, Cr)Te with interstitial impurities, such as Li, Na and Cu, from first-principles by using the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. From the total energy results, it is shown that the mixing energy of magnetic impurity becomes negative and the solubility of magnetic impurities is strongly enhanced under the existence of interstitials [1]. In general, the co-dopants compensate hole carriers, thus the system becomes paramagnetic. However, owing to the large diffusivity of these interstitial impurities, we can anneal out the co-dopants after the crystal growth to recover the ferromagnetism. As an example, kinetic Monte Carlo simulations for the diffusion of interstitial co-dopants in DMS will be shown. [1] K. Sato et al., Jpn. J. Appl. Phys. 46 L1120 (2007)

Time Resolved Spectroscopy of InMnAs Using Differential Transmission Technique in Mid-Infrared Region. M. BHOWMICK, K. NONTAPOT, G.A. KHODAPARAST, Physics Department, Virginia Tech., B.W. WESSELS, Materials Research Center, Northwestern University — The emergence of III-Mn-V magnetic semiconductors, such as GaMnAs, InMnAs, and InMnSb has led to a number of exciting results relevant to the new field of spintronics. In contrast to earlier MBE work, InMnAs structures grown by MOVPE at the Northwestern University are room temperature ferromagnetic with a $T_C$ of 330 K. The origins of ferromagnetism and the interactions between itinerant carriers and localized spins in these structures are open and interesting questions. The samples are grown on GaAs substrates with the Mn content ranging from 0-1.4%. The carrier and spin life times in these structures are probed using a differential transmission technique by tuning the pump-probe radiation from 3-3.6 microns. The relaxation times are in order of 2-4 ps similar to the observations in the MBE grown structures. The temperature dependence of the carrier and spin lifetimes will be presented and related to recent models for spin recombination.

Supported by: NSF-DMR-0507866, NSF-DMR 0804170, AFOSR Young Investigator Program 06E231.

Wednesday, March 18, 2009 11:15AM - 2:15PM – Session Q23.00002 The quenching of scattering-enhanced tunneling in the Quantum Hall Regime. KASEY RUSSELL, FEDERICO CAPASSO, VENKATESH NARAYANAMURTI, Harvard University, HONG LU, JOSHUA ZIDE, ARTHUR GOSSARD, UC Santa Barbara — Using capacitance-voltage spectroscopy, we are able to probe the magnetic field dependence of the quasi-bound state lifetime of a quantum well. Our measurements are done on a special InGaAs/InAlAs heterostructure that is designed to promote scattering-enhanced tunneling out of the quantum well. The bound state lifetime shows large oscillations as the magnetic field is varied, which result from the quenching of electron scattering as the Fermi level crosses a Landau Level. The results are interpreted in terms of the edge states and cyclotron orbits of the Integer Quantum Hall Effect.
11:39AM Q23.00003 Microwave modes of a two-dimensional electron systems in the presence of a perpendicular magnetic anisotropy provided by a macroscopic ferromagnet. BRENDEN MAGILL, NHMFL and MARTECH, FSU, L. W. ENGEL, NHMFL/FSU, M. P. LILLY, J. A. SIMMONS, J. L. RENO, Sandia National Laboratory — We report on a resonance in the microwave absorption spectrum of a high mobility two dimensional electron system (2DES) in a spatially varying magnetic field from a ferromagnet placed near the sample. The ferromagnet, made of Dy, cylinder or plates, with a hole through it. Microwave transmission between contacts capacitively coupled to the 2DES near the hole or cylinder shows a resonant absorption peak $f_{pk}$ for holes and cylinders with varying radii, $r_m$, from 0.5 mm to 125 mm. The resonance absorption is present for a uniform external field $B_0$ less than 1 T and only for specific magnitization of the ferromagnet with respect to $B_0$ with $f_{pk}$ decreasing as either $B_0$ or $r_m$ increase. We will interpret the data in terms of plasma excitations similar to edge magnetoplasmons [1] confined along the magnetic field inhomogeneity by the large magnetic field gradients there. [1] See, for example, V. A. Volkov and S. A. Mikhailov, Sov. Phys.-JETP 67, 1639(1988).

11:51AM Q23.00004 Itinerant electron-driven chiral magnetic ordering and spontaneous quantum Hall effect in triangular lattice models. IVAR MARTIN, C.D. BATISTA, Theoretical Division, Los Alamos National Laboratory — We study the Kondo Lattice and the Hubbard models on a triangular lattice. We find that at the mean field level, these rotationally invariant models naturally support a non-coplanar chiral magnetic ordering. It appears as a weak-coupling instability at the band filling factor 3/4 due to the perfect nesting of the itinerant electron Fermi surface. This ordering is a triangular-lattice counterpart of the collinear Neel ordering that occurs on the half-filled square lattice. While the long-range magnetic ordering is destroyed by thermal fluctuations, the chirality can persist up to a finite temperature, causing a spontaneous quantum Hall effect in the absence of any externally applied magnetic field.

12:03PM Q23.00005 Comparative study of radiation-induced transport in Wegscheider’s and Umansky’s GaAs/AlGaAs material. 1, 2 R.G. MANI, Georgia State University, W. WEGSCHEIDER, Univ. of Regensburg, V. UMANSKY, Weizmann Inst. — Transport studies of GaAs/AlGaAs specimens have shown radiation-induced, periodic-in-the-inverse-magnetic-field, magnetoresistance oscillations that saturate into novel radiation-induced zero-resistance states (RIZRS) at the deepest oscillatory minima.[1] The origin of these RIZRS remains a topic for further experimental investigation, as does the dependence of these phenomena on the impurity configuration and the material quality. On the latter point, it remains to be understood if similar material prepared in different laboratories yield a similar response under the same conditions. In addressing this issue, we examine here the radiation-induced transport in GaAs/AlGaAs material prepared by W. Wegscheider and co-workers. In a previous study, Simovic et al.[2] have reported the observation of B-periodic radiation-induced oscillations and the strong suppression of the inverse-B periodic oscillations in Wegscheider’s GaAs/AlGaAs material. Here, we compare our experimental results to their study and also to our own previous results obtained on specimens prepared by V. Umansky and co-workers. 1) R. G. Mani, Appl. Phys. Lett., 91, 132103 (2007). 2) B. Simovic et al., Phys. Rev. B 71, 233303 (2005).

12:15PM Q23.00006 Transport measurements and simulations of GaAs/AlGaAs “anti-Hall-bar within a Hall bar” devices. ANNIKA KRIISA, Emory University, RAMESH G. MANI, Georgia State University — Hall effect measurements are often carried out in the Hall geometry, which is a thin rectangular plate with current and Hall voltage contacts at the external boundary. The motivation of this study is to further understand the impact on Hall effect when a hole is inserted inside Hall geometry. One way on conducting this investigation is to superimpose an “anti-Hall bar” inside the standard Hall bar, where the anti Hall bar is actually the hole inside the Hall device with contacts on the inside boundary of this hole. This configuration is thought to generate an ordinary Hall effect within the interior boundary such that the interior Hall voltage divided by the interior injected current equals the Hall resistance. One believes that it might also be possible to simultaneously realize multiple independent Hall effects by injecting multiple currents into the multiply connected device [1]. We have studied Hall effect in the doubly connected “anti-Hall bar within a Hall bar” geometry fabricated out of the GaAs/AlGaAs semiconductor system. Also the simulations of the distribution of the Hall current and potential profile within the specimen are conducted. To attain understanding of how the Hall effect arises in this geometry, the simulation plots are compared to the experimental results.

12:27PM Q23.00007 Effect of strain on nematic phases of two-dimensional hole gases. SUNANDA KODUVAYUR, LEONID ROKHINSON, Purdue University, MICHAEL MANFRA, Bell laboratories, Lucent Technologies — We study the effect of uniaxial strain on high Landau levels(LL). $N \geq 2$ (N is the LL index), in two dimensional hole gases(2DHG). The presence of anisotropic magnetotransport at certain half-integer filling factors in these systems has been understood as a signature of stripe or nematic phases. Recent studies on 2DHG in a perpendicular field have shown anisotropic transport at filling factors $\nu = 7/2$ and 11/2 accompanied by an isotropic 9/2 state. These results differ from those of 2D electrons where anisotropy is only observed for LLs with $N \geq 3$. While this difference has been attributed to stronger spin-orbit interactions in holes, the origin and conditions for the stabilization of these states are still open questions. We study samples fabricated in the Van der Pauw geometry from C-doped GaAs/AlGaAs 2DHG grown on (001) substrate. We apply uniaxial strain along [110] and study the transport properties in a perpendicular field at 10mK. We introduce nematic states earlier on for $2 \leq N \leq 7$ with large enough strain. Furthermore, we demonstrate reversal in direction of anisotropy at filling factors $\nu = 7/2$ and 5/2 with strain modulation. We also see a difference in strain response of the resistance along [110] and [110]. We try to understand the observed effects using an electrostatic model which incorporates the anisotropy of the elastic moduli of GaAs.

12:39PM Q23.00008 Dependence of Effective Mass on Spin and Valley Degrees of Freedom. MANSOUR SHAYEGAN, TAYFUN GOKMEN, MEDINI PADMANABHAN, Dept. of Electrical Engineering, Princeton University, Princeton, NJ 08544 — We measure the effective mass ($m^*$) of interacting two-dimensional electrons confined to an AlGaAs quantum well at a fixed density while we change the conduction-band valley occupation and the spin polarization via the application of strain and magnetic field, respectively [1]. Compared to its band value, $m^*$ is enhanced when the electrons are valley or spin unpolarized, and the largest enhancement is observed for the case where both spin and valley are unpolarized. Consistent with the study of M. Padmanabhan et al., in the fully spin- and valley-polarized regime, the measured $m^*$ is suppressed compared to the band value. Incidentally, in the fully spin- and valley-polarized regime, the electron system exhibits an insulating behavior. [1] T. Gokmen et al., Phys. Rev. Lett. 101, 146405 (2008). [2] M. Padmanabhan, et al., Phys. Rev. Lett. 101, 026402 (2008).

12:51PM Q23.00009 Anomalous Effective Mass of Two-dimensional Holes in a Strong Parallel Magnetic Field. YENTING CHIU, MEDINI PADMANABHAN, JAVAD SHABANI, MANSOUR SHAYEGAN, Department of Electrical Engineering, Princeton University, ROLAND WINKLER, Department of Physics, Northern Illinois University — We report effective hole mass ($m^*$) measurements through analyzing the temperature dependence of the Shubnikov-de Haas oscillations in dilute (density $\sim 5\times10^{10}$cm$^{-2}$) two-dimensional (2D) hole systems confined to a 20nm-wide, (311)A GaAs quantum well. In this system the 2D holes occupy two spin-subbands whose $m^*$ we measure to be $\sim 0.2$ (in units of free electron mass), in good agreement with the theoretical band calculations. We then apply a sufficiently strong ($>10T$) parallel magnetic field to fully depopulate one of the spin subbands, and measure $m^*$ for the populated subband. We find that this latter $m^*$ is close in magnitude to the $m^*$ we measure in the absence of the parallel field. This is a surprising observation as it is in stark disagreement with the results of our band calculations which take into account the spin-orbit interaction and the holes’ finite layer thickness, and predict a large enhancement of $m^*$ in a strong parallel magnetic field.
n=12 and was most sensitive at the filling fraction n=6.

We have also characterized the SET magnetometer by an ac technique where we applied 170 nT ac magnetic fields to monitor the conductance of the SET following a small change in magnetic field, we studied the equilibration processes in IQHLs. The equilibration times are found to be strongly dependent on the magnetic field and became unmeasurably long (many days) as we decreased T down to ~0.4 K and its downturn at lower temperatures, is in agreement with the theory. The values of the Fermi-liquid parameter obtained from the comparison agree with the corresponding values extracted from the analysis of Shubnikov–de Haas oscillations based on the theory of magneto-oscillations in interacting 2D systems [4].

Supported by the BSF grant No. 2006201

### 2:03PM Q23.00010 Quantum Hall Effect and Field Dependent Valley Splitting on High Mobility Silicon-(111) Surfaces

TOMASZ M. KOTT, ROBERT N. McFARLAND, LUYAN SUN, BRUCE E. KANE, Laboratory for Physical Sciences, University of Maryland, College Park, KEVIN ENG, Sandia National Laboratories — We have developed a method for fabricating field effect transistors, using vacuum as the dielectric, in order to study electron transport on a clean, flat, chemically prepared hydrogen-terminated surface. Resulting devices display high mobilities (100,000 cm²/V s at 70 mK), enabling us to probe field dependent transport dynamics of this six-fold valley degenerate surface. We will present evidence that a low oxygen environment during sample preparation is necessary to achieve high mobilities. To support the correlations between surface chemistry and electronic properties, we will show AFM images of the surface for various preparation techniques. Finally, we will describe high field magneto-transport measurements (up to 12 T) indicate field-dependent valley splitting. In particular, we find easily resolvable filling factors of, amongst others, 3, 5, and 7, an indication that the six-fold degeneracy is possibly broken by many-body effects. I will also show preliminary data with hints of the FQHE at ν = 3/2.

### 1:15PM Q23.00011 Interaction Effects in Conductors of a Two-Valley Electron System in High-Mobility Si Inversion Layers

NIKOLAI N. KLIMOV, Rutgers University, DMITRY A. KNYAZEV, OLEG E. OMEL’YANOVSKI, VLADIMIR M. PUDALOV, Lebedev Physical Institute, HARRY KOJIMA, MICHAEL E. GERSHENSON, Rutgers University — We have measured the conductivity of high-mobility (100) Si metal-oxide-semiconductor field-effect transistors over wide ranges of electron densities n = (1.8−15) × 10¹¹ cm⁻², temperatures T = 30 mK−4.2 K, and in-plane magnetic fields Bₚ = 0−5 T [1]. The experimental data have been analyzed using the theory of interaction effects [2] in the conductivity of disordered two-dimensional (2D) systems. The parameters essential for comparison with the theory, such as the intervalley scattering time and valley splitting, have been measured or evaluated in independent experiments [1,3]. The observed behavior of σ, including its quasi-linear increase with decreasing T down to ~0.4 K and its downturn at lower temperatures, is in agreement with the theory. The values of the Fermi-liquid parameter obtained from the comparison agree with the corresponding values extracted from the analysis of Shubnikov–de Haas oscillations based on the theory of magneto-oscillations in interacting 2D systems [4].

### 1:27PM Q23.00012 2DEG effect on vibration of piezoelectric plates

ALEXEY SUSLOV, National High Magnetic Field Laboratory, Tallahassee, FL — Resonances of a GaAs wafer with a GaAs/AlGaAs heterostructure grown on one of its sides were studied in the temperature range 0.05-10 K in magnetic fields of up to 18 T. To the best of our knowledge, this is the first use of the Resonant Ultrasound Spectroscopy in a dilution refrigerator. Observed quantum oscillations of the resonance frequencies and linewidths were caused by the Quantum Hall Effect in the 2DEG. The wafer with the 2D gas can be conceived as a film with field dependent conductivity deposited on a piezoelectric plate. Being dielectric, the film does not affect properties of GaAs and, thus, the resonance frequencies are defined only by the elastic, piezoelectric, and dielectric constants of GaAs. Being metallic, the 2D sheet effectively screens the parallel electric field, so the ultrasound wave velocities and resonance frequencies decrease with the increase of the sheet conductivity. Oscillations of the resonance linewidth reflect the influence of the 2D system on the ultrasound attenuation. A metallic film as well as a dielectric one does not affect this attenuation but at some finite nonzero value of the conductivity the linewidth approaches a maximum value. The observed phenomena can be described by the relaxation type equations.

### 1:39PM Q23.00013 Quantum Hall transition on a triangular lattice; network model and analytical renormalization-group treatment

VAGHARSH MKHITARYAN, MIKHAIL RAIKH, Department of Physics, University of Utah, Salt Lake City, UT 84112 — Common approach to the theoretical study of the quantum Hall transition is the Chalker-Coddington network model on the square lattice. We introduce a new version of the network model formulated on the triangular lattice, where the scattering at the sites is described by a 3 × 3 matrix. Extending renormalization-group description of the classical site percolation to the quantum case, we derive a closed equation for the distribution function of conductance. Solving this equation numerically, we get for the critical exponent of the correlation radius ν ≈ 2.3 ± 0.76 in good agreement with established value ν = 2.33.

### 1:51PM Q23.00014 Half integer features in the quantum Hall Effect: experiment and theory

TOBIAS KRAMER, University Regensburg, E.J. HELLER, R.E. PARROTT, Harvard University, C.T. LIANG, National Taiwan University, C.F. HUANG, National Measurement Laboratory, Taiwan, K. Y. CHEN, National Taiwan University, L.-H. LIN, National Chiayi University, Taiwan, J.-Y. WU, S.-D. LIN, National Chiao Tung University, Taiwan — We discuss experimental data and a new model of the quantum Hall effect (IQHE), which explains an intriguing substructure within Landau levels observed at higher currents. The experiments show inflection points in the Hall resistivity around filling factors 5/2 and 7/2. The experiments require to revisit the foundations of the IQHE and to establish an injection model which incorporates the correct boundary conditions imposed by a real Hall device and the Lorentz force. We have to follow the electrons to their source: one corner of the Hall bar and its steep electric field gradients, rather than focusing on the middle of the Hall device. We find the entire Hall resistivity curve is calculable as a function of magnetic field, temperature, and current. In contrast to previous theories of the IQHE, disorder plays no fundamental role in our theory. Contrary to the standard picture of Landau levels in disorder system, we predict and observe gaps right in the middle of certain Landau levels. The Hall plateaus and half integer inflections are shown to result from the LDOS appropriate to the magnetic field and the strong electric field at the injection corner.

### 2:03PM Q23.00015 Operation of a Single Electron Transistor Placed on Stacked Integer Quantum Hall Layers as a Magnetometer

HAILING CHENG, YU JIN, Physics Dept., Univ. of Michigan, RACHEL GOLDMAN, Dept. of Materials Science and Engineering, Univ. of Michigan, CAGLIYAN KURDAK, Physics Dept., Univ. of Michigan — A single electron transistor (SET) placed on an integer quantum Hall liquid (IQHL) can detect small time varying magnetic fields in the presence of a large constant magnetic field. To enhance the sensitivity, we placed a SET made out of Al/AlOₓ/Al tunnel junctions on top of a GaAs/AlGaAs heterostructure with 25 identical quantum well structures. By monitoring the conductance of the SET following a small change in magnetic field, we studied the equilibration processes in IQHLs. The equilibration times associated with small changes in magnetic field are found to be strongly dependent on the magnetic field and became unmeasurably long (many days) as we got closer to the center of the quantum Hall plateaus. We have also characterized the SET magnetometer by an ac technique where we applied 170 nT ac magnetic field and measured the response of the SET using a double lock-in technique. At T=20 mK, the SET magnetometer worked at filling fractions up to n=12 and was most sensitive at the filling fraction n=6.

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Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q24 DMP: Focus Session: Optical Response of Nanotubes
11:15AM Q24.00001 Optical near-field investigations of individual single-walled carbon nanotubes1, ACHIM HARTSCHUH, LMU Muenchen — Optical excitation of semiconducting nanotubes creates excitons that determine nearly all light-based applications. Near-field photoluminescence (PL) and Raman imaging with a spatial resolution better than 15 nm was used to probe the spectroscopic properties of excitonic states along single nanotubes on substrates [1,2]. The PL intensity was found to decrease towards the nanotube ends on a length scale of few 10 nm probably caused by exciton transport to localized end states followed by efficient non-radiative recombination. DNA-wrapping of nanotubes results in pronounced emission energy variations on a length scale of few 10 nm indicating the potential of the material for nanoscale sensing applications [3]. Inter-nanotube energy transfer was studied for different pairs of semiconducting nanotubes forming bundles and crossings [4]. Efficient transfer is found to be limited to a few nanometres because of competing fast non-radiative relaxation and can be explained in terms of electromagnetic near-field coupling. We also report on our recent experimental results on time-resolved near-field PL measurements, electrically gated nanotubes and the PL of nanotubes on metal surfaces.

References:

1Financial support by the DFG through grant HA4405/4-1 and Nanosystem Initiative Muenchen (NIM) is gratefully acknowledged.

11:51AM Q24.00002 Electroluminescence Spectral Shape in Carbon Nanotube Field Effect Transistors under High Bias Conditions, MEGUMI KINOSHITA, Stony Brook University, VASILI PEREBEINOS, MATHIAS STEINER, PHAEDON AVOURIS, IBM THOMAS WATSON RESEARCH CENTER TEAM — In carbon nanotube field effect transistors, electroluminescence excited by intra-nanotube impact excitation at high source-drain bias reveals strongly broadened electronic transitions (FWHM ~150 to ~300 meV for the lowest energy peak observed) in the E1g to E2g energy range. Through the bias and polarization dependence of the spectra, we investigate the production mechanism of these states and consider possible causes for their bias-dependent broad line shapes, including exciton-exciton annihilation and high electron and phonon temperatures.

12:03PM Q24.00003 Electroluminescence from Carbon Nanotube Network Transistors, ELYSE ADAM, CARLA AGUIRRE, Departement de Genie Physique, Ecole Polytechnique de Montreal, MATTHIEU PAILLET, Departement de Chimie, Universite de Montreal, BENNOID CARDIN ST-ANTOINE, Departement de Genie Physique, Ecole Polytechnique de Montreal, FRANCOIS MEUNIER, Departement de Chimie, Universite de Montreal, PATRICK DESJARDINS, DAVID MENARD, Departement de Genie Physique, Ecole Polytechnique de Montreal, RICHARD MARTEL, Departement de Chimie, Universite de Montreal — A spectroscopic study of the electroluminescence properties of individual carbon nanotube (CNFET) and carbon nanotube network (NNFET) field effect transistors has been performed. As expected, the measurements on metallic and semiconducting CNFET showed that only semiconducting carbon nanotubes produce electroluminescent signals. The narrow emission line widths of CNFET (~80 meV) compared to that of NNFETs (~180 meV) indicates that the light emission from carbon nanotube networks involves many carbon nanotubes. Moreover, electroluminescence spectra from NNFETs made from three different sources of carbon nanotubes (laser ablation, CoMoCAT and DWNT) have shown major differences which, based on comparisons with their corresponding absorption spectra, indicate that only larger diameter carbon nanotubes contribute to light emission.

12:15PM Q24.00004 Confocal imaging and excitation spectra of photoluminescence from carbon nanotubes suspended over trenches of various widths1, S. MORITSUBO, T. MURAI, T. SHIMADA, Y. MURAKAMI, S. MARUYAMA, Y. K. KATO2, University of Tokyo — Carbon nanotubes (CNTs) have novel optical properties, such as strongly bound excitons and sensitivity to surrounding environments, because of their unique structure. In particular, it is well known that CNTs lying on substrates show photoluminescence (PL) quenching caused by very effective substrate-induced nonradiative decay of photoexcited excitons. In this study, we formed trenches with various widths on SiO2/Si substrates in order to prepare suspended CNTs. Using ethanol as carbon source, chemical vapor deposition was used for the synthesis of CNTs. PL images were collected by a home-built laser scanning confocal microscope system utilizing a fast staring mirror. In addition, PL excitation spectra were taken using a wavelength tunable Ti:sapphire laser. We analyzed these PL images and excitation spectra in order to clarify the interaction between excitons and the substrate.

1This work was supported by JST PRESTO and KAKENHI programs.
2PRESTO, Japan Science and Technology Agency

12:27PM Q24.00005 Near infrared photoresponse study of large area multi-walled carbon nanotube film with different electrode spacing, BIDDUT SARKER, M. ARIF, PAUL STOKES, ALAMGIR KABIR, SAIFUL I. KHONDAKER, Nanoscience Technology Center and Department of Physics University of Central Florida, Orlando, FL 32826 — Photoconductivity of carbon nanotube has generated considerable debate in terms of whether the photoresponse is (i) due to photon induced charge carrier (excitonic), (ii) due to heating of the CNT network (bolometric), or (iii) caused by photodesorption of oxygen molecules at the surface of the CNT. In addition, the role of the metal electrode – CNT contact’s effect on the photoresponse has also been debated. In this talk, we will present near-infrared photoresponse study of multi-walled carbon nanotube (MWCNT) film with different electrode spacings. We found that there is a large enhancement of photocurrent upon laser illumination and the photocurrent strongly depends on the position of the laser spot with maximum response occurring at the metal – film interface. We also show that the photoresponse is rather slow (~1s) and increases with increasing electrode spacing. We will discuss the origin of the position dependent photocurrent and slow time response.

12:39PM Q24.00006 Transparency and conductivity of carbon nanotube networks, JAN OBRZUT, National Institute of Standards and Technology — The conductivity of films made of single wall carbon nanotubes longer than 200 nm closely follows the percolation theory for two-dimensional (2D) networks. The scaling universal exponents describing the “percolation” transition from an insulating to conducting state with increasing concentration are consistent with 2D percolation model. A sheet of tubes about 820 nm long becomes conducting at an amazingly low concentration of about 1.2×10^-9 g/cm^2. In comparison, batches of short nanotubes or mixed-length batches form more 3D networks that conduct noticeably worse. Furthermore, the conductivity percolation threshold (x_c) varies with the aspect ratio Length (L) as, x_c ~L/L, a result that is also in accordance with the percolation theory. We also show that contrary to current predictions, these sheets do not have optical properties similar to thin metallic films. Our results indicate that the correlation between the optical properties and the electrical conductivity of these sheets is again better predicted by the general percolation theory.
12:51PM Q24.00007 Carrier renormalization effects on the optical response of doped semiconducting single-walled-carbon nanotubes1, SHENG JU, Department of Physics, University of California, Berkeley, California 94720, USA, CHEOL-HWAN PARK, STEVEN LOUIE, Department of Physics, University of California, Berkeley, California 94720, USA and Materials Science Division, Lawrence Berkeley National Laboratory — It is known that many-electron effects dramatically change the optical properties of single-walled carbon nanotubes (SWCNTs). Recently, researchers have succeeded in tuning the Fermi energy of an individual SWCNT by applying a gate voltage or by introducing adsorbate dopants. Therefore, the optical response of doped SWCNTs is not only interesting from a pure scientific viewpoint but also important for the application of these systems. We present here first-principles calculations, based on the GW-Bethe Salpeter equation (GW-BSE) approach, of the quasiparticle (single-particle excitation) spectrum and the electron (electron-hole excitation) spectrum of doped SWCNTs.

1This research was supported by the NSF under Grant No. DMR07-05941, and the U.S. DOE under Contract No. DE-AC02-05CH11231. Computer time was provided by NERSC and NPACI.

1:03PM Q24.00008 Optical properties of doped semiconducting single-walled carbon nanotubes. CATALIN D. SPATARU, FRANCOIS LEONARD, Sandia National Laboratories, Livermore, CA 94551 — We studied how the optical response of semiconducting single-walled carbon nanotubes (SWCNTs) changes upon doping. We performed ab initio calculations of the optical absorption spectrum of the p-doped (10,0) SWCNT, employing a many-electron Green’s function approach that determines both the quasiparticle and electron-hole excitations from first principles. We found that the absorption spectrum changes dramatically upon doping, due to both quasiparticle and excitonic effects. In the independent quasiparticle picture, the electron-hole continua are strongly red-shifted with respect to the undoped case due to the metallic character acquired by the electronic screening upon doping. However, the main optical features in the absorption spectrum, including both quasiparticle and electron-hole interaction effects, are only slightly shifted, but qualitatively very different, with respect to the undoped case. Small doping levels (where the Fermi level lies below the valence band maximum by an energy much smaller than the binding energy of excitons in the undoped SWCNT) are sufficient to bleach band-gap absorption. In addition, while resonant excitons associated with the second electron-hole continuum can still exist in the doped SWCNT, their binding energy is much reduced, to a level typical of metallic SWCNTs of similar diameter.

1:15PM Q24.00009 Origins of optical absorption components of metallic and semiconducting single-wall carbon nanotubes in ultra-violet region, KAZUHIRO YANAGI, TAKESHI SAITO, YASUMITSU MIYATA, HIRONICHI KATAURA, Natl. Inst. Adv. Indus./Sci. Tech. — There are large absorption components in the optical absorption spectra of single-wall carbon nanotubes (SWCNTs) in the ultraviolet (UV) region (~5 eV). Clarification of the origins of the UV absorption is important, since the tails of the UV components influence the transparency of nanotubes and impede their uses for transparent conducting films. However, the origins have not been correctly understood yet. Such UV absorption components are assumed to be caused by π-plasmons, however, recently contributions from π−π* transition at the M point were also suggested. To understand the origins of UV component, here we clarified how the electronic structure (metallic or semiconducting) and the diameters of SWCNTs influence the UV optical absorption features. We clearly identified two components in UV region, and revealed dependence of the components on their diameters. Remarkably, dependence of the peak-energies of one component on diameters could not be explained by plasmon model, implying the presence of different origins than plasmons in the UV absorption components.

1:27PM Q24.00010 Environmental Change in UV Absorption by Single-Walled Carbon Nanotubes, YOICHI MURAKAMI, SHIGEO MARUYAMA, Univ. of Tokyo — We investigated the UV absorption of single-walled carbon nanotubes (SWNTs) in the 4 - 6 eV range, which has been customarily referred to as the “π-plasmon” as a whole. The optical absorption spectra of aligned SWNTs were measured in different dielectric environments. The experimental results unambiguously show that, for the two different UV absorption components existing in the 4 - 6 eV range, only the feature at 5.0 - 5.3 eV exhibits remarkable spectral changes, while the other feature at ~4.5 eV remains unchanged. We attribute the former (5.0 - 5.3 eV) to a dipolar surface plasmon in the radial direction of SWNTs. On the other hand, the experimental result raises a fundamental question as to whether it is appropriate to classify the UV feature at ~4.5 eV as a π-plasmon. We will discuss its relation with the UV absorption at ~4.5 eV in graphite/graphene that has long been recognized as the interband transition at M point of the Brillouin Zone.

1:39PM Q24.00011 Electron-electron interaction effects on the photophysics of metallic single-walled carbon nanotubes1, SUMIT MAZUMDAR, University of Arizona, DEMETRA PSIACHOS, ZHENDONG WANG, ROBERTO BADILLA, University of Arizona — Within a molecular Hamiltonian appropriate for correlated π-electron systems, we show that optical excitations polarized parallel to the nanotube axes in the so-called metallic single-walled carbon nanotubes are to excitons. Our calculated absolute exciton energies in twelve different metallic single-walled carbon nanotubes, with diameters in the range 0.8 - 1.4 nm, are in nearly quantitative agreement with experimental results. We have also calculated the absorption spectrum for the (21,21) single-wall carbon nanotube in the E22 region. Our calculated spectrum gives an excellent fit to the experimental absorption spectrum. In all cases our calculated exciton binding energies are only slightly smaller than those of semiconducting nanotubes with comparable diameters. As in the semiconducting nanotubes we predict in the metallic nanotubes a two-photon exciton above the lowest longitudinal polarization exciton that can be detected by ultrafast pump-probe spectroscopy. We also predict a subgap absorption polarization perpendicular to the nanotube axes below the lowest longitudinal exciton, blueshifted from the exact midgap by electron-electron interactions.

1This work was supported by NSF grant number DMR-0705163.

1:51PM Q24.00012 Fano Resonance in Single-Walled Cabron Nanotube Devices, GANG LIU, University of California, Riverside, YONG ZHANG, China Southwest University, CHUNNING LAU, University of California, Riverside — We have observed Fano resonance in a short carbon nanotube device. The device’s transport spectroscopy exhibits inverse Coulomb blockade structures superimposed on Fabry Perot resonance patterns, indicating the quantum interference between a well-coupled channel and a poorly-coupled channel. Our results have implication on the detection of charges’ phase and phase coherence in an electronic interferometer.

2:03PM Q24.00013 Optical Absorption Spectra of Charge Doped Single-Walled Carbon Nanotubes from First-principles Calculations, GUANGFU LUO, Department of Physics, Peking University, JING LU, WAI-NING MEI, LU WANG, LIN LAI, JING ZHOU, RUI QIN, HONG LI, ZHENGXIAN GAO, DEPARTMENT OF PHYSICS, PEKING UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION — The optical absorption spectrum of single-walled carbon nanotubes (SWCNTs) under charge doping is often interpreted within the graphene zone-folding and rigid-band model. Based on the periodic boundary model together with a uniform background countercharge, our density functional theory calculations, however, show that the spectrum response deviates from the expectations of such model. Specifically, the SWCNT band structures can differ qualitatively from the zone-folding ones, and with the increasing doping level, the absorption peaks will bleach in a non-sequential energy order. The on-tube bands in SWCNTs sometimes change obviously even under low charge doping level, and accordingly cause spectra peaks to shift, split, and merge. At the end of this paper, we discuss briefly the applicability of the present results at the GW-BSE theory level and in other SWCNT-like systems.
11:15AM Q25.00001 Interaction of magneto-excitons with phonons in graphene and graphite
JUN YAN, TREvor DAVId RHONE, Department of Physics, Columbia University, SARAH GOLER, NEST and Scuola Normale Superiore, Pisa, Italy, MELINDA HAN, Department of Physics and Applied Physics, Columbia University, VITTORIO PELLEGRINI, NEST and Scuola Normale Superiore, Pisa, Italy, PHILIP KIM, Department of Physics, Columbia University, ARON PINCZUK, Department of Physics and Applied Physics, Columbia University — We study the Landau levels of graphite and single layer graphene by measurements of the magneto-phonon resonance effect in which there is coupling between the inter-Landau level magneto-exciton with the long wavelength optical phonon (G band). In graphite the G band displays a rich line shape evolution as the magnetic field is finely tuned between 5 and 7 Tesla. These observations indicate that the G band is resonantly coupled to the magneto-excitons at these fields. In the interpretation we postulate that the anticrossing of the phonon band with the inter-Landau level transitions results in a mode-splitting at around 6.2 T. The evolution of the energy and spectral weight of the two coupled modes indicates that the phonon is a probe of the unique structure of Landau levels in graphene-related materials. In an as-prepared single-layer graphene, much smaller changes are observed for fields reaching as high as 12 Tesla.

11:27AM Q25.00002 Klein Backscattering and Fabry-Perot Interference in Graphene Heterojunctions, ANDREI SHYTVO, University of Utah, MARK RUDNER, Harvard University, LEONID LEVITOV, Massachusetts Institute of Technology — Fabry-Perot (FP) interference in a lateral p-n-p structure in graphene is proposed as a vehicle to probe Klein scattering phenomenon [Phys. Rev. Lett. 101, 156804 (2008)]. In ballistic regime, interference between waves scattered from p-n interfaces leads to oscillations in conductance as a function of electron density. Perfect transmission at zero incidence angle (Klein effect) implies a sign change of the backreflection amplitude. This change contributes a phase π to interference and shifts FP fringes by half a period. Alternatively, the π phase can be understood as Berry's phase accrued by electron bouncing between p-n boundaries. This effect is revealed in the evolution of fringes when a relatively weak, non-quantizing magnetic field is applied. The behavior of the interference fringes recently observed by Young and Kim (arXiv:0808.0855) is consistent with this picture. The observed crossover to Shubnikov-de Haas oscillations can be also understood from quantization of periodic orbits bouncing between the two p-n interfaces.

11:39AM Q25.00003 Graphene electronics via strain engineering, VITOr PEREIRA, Boston University — Recently, graphene has been confirmed as the strongest material ever measured, being able to sustain reversible deformations in excess of 20%. These mechanical measurements arise at a time where graphene draws considerable attention on account of its unusual and rich electronic properties. Besides the great crystalline quality, high mobility and resilience to high current densities, they include a strong field effect, absence of backscattering and a minimum metallic conductivity. While many such properties might prove instrumental if graphene is to be used in future technological applications in the ever pressing demand for miniaturization in electronics, the latter is actually a strong deterrent: it hinders the pinching off of the charge flow and the creation of quantum point contacts. In addition, graphene has a gapless spectrum with linearly dispersing, Dirac-like, excitations. Although a gap can be induced by means of quantum confinement in the form of nanoribbons and quantum dots, these “paper-cutting” techniques are prone to edge roughness, which has detrimental effects on the electronic properties. We explore an alternative route for tailoring the electronic structure of graphene, based on a strain engineering. We will discuss how local and global strain profiles can be suitably tailored to impact the bandstructure of graphene and control its transport characteristics. Electron confinement, electron beam collimation, energy filtering, surface modes and bulk spectral gaps are some examples of what might be achieved.

11:25AM Q25.00004 Fabrication and transport measurement of suspended graphene devices.
WENZHONG BAO, FENG MIAO, GANG LIU, CHUNNING LAU — We developed a lithography-free technique to fabricate suspended graphene devices. Graphene sheets are exfoliated over pre-defined trenches over the substrates, and electrodes are deposited via shadow mask evaporation. This technique eliminates resist residues which may affect electrical properties of graphene. We will discuss results from electrical transport measurement at different temperatures and magnetic fields.

11:27PM Q25.00005 Temperature dependent resistivity of suspended graphene, EROS MARIANI, FELIX VON OPPEN, Freie Universitaet Berlin, FREIE UNIVERSITAET BERLIN TEAM — In this talk we discuss the temperature dependence of the resistivity for suspended single layer graphene, due to electron-phonon scattering. All the temperature regimes are studied, as well as the contributions due to the different acoustic phonon branches in graphene. We show how tension in the membrane suppresses the otherwise dominant contribution due to flexural phonons [1], leaving a linear temperature scaling compatible with recent experiments. The eventual crossover to quadratic temperature dependence at very high temperatures could be used as an experimental tool to investigate the otherwise unknown strength of the tension. Finally, we discuss the transition to the quasi-nondegenerate regime for electrons in graphene. This is relevant for current experiments on the temperature dependent resistivity in most temperature regimes, and can shed light on the unexpected density dependence of the linear-T resistivity.


12:39PM Q25.00006 Neutron Scattering Studies of Graphene, ALICE ACATRINEI, ZHIJUN LIN, LUKE DAEMEN, Los Alamos National Laboratory, LANSCe, Lujan Neutron Scattering Center — We synthesized graphene by thermal exfoliation at 500 deg C. The material is nanosize, as confirmed by TEM/SEM, with flake transverse dimensions 50-100 nm. We present the first detailed measurement of the vibrational Spectrum of both graphene and graphite using INS, along with a neutron Scattering study of hydrogen adsorbed on graphene. Our measurements were collected at 10K using the Filter Difference Spectrometer (FDS) at Lujan Neutron Scattering Center, Los Alamos National Laboratory.

12:51PM Q25.00007 Effect of film corrugation on the optical phonon lifetime in graphene, PETER EKLUND, Department of Physics, Department of Material Science and Engineering, Pennsylvania State University, University Park, PA 16802, AWWING GU, Department of Materials Engineering, Pennsylvania State University, University Park, PA 16802 — We present results of a microRaman study of n-layer graphene films supported on ~atomically flat mica, Si/SiO₂ (or varying roughness) and suspended above a trench. Using the Raman G-band line width Γ₂G, we find that the optical phonon lifetime τ ~1/Γ₂ decreases linearly with increasing rms substrate roughness δ, and independent of the chemical composition of the substrate. In agreement with this general observation, we find that Γ₂ for unsupported graphene is significantly higher (i.e., the q=0 optical phonon lifetime is significantly lower) than observed when the film is supported on mica. Correlating Γ₂ with values obtained from supported films, we infer an inherent rms roughness δ ~ 2 nm for unsupported graphene, in reasonable agreement with recent STM reports that first suggested that graphene might prefer to spontaneously convert to a corrugated system. Our observations may then relate to the effect of the local bending of the sp² sheet on the electron-phonon interaction.
1:03PM Q25.00008 Edge stress induced warping of graphene sheets and nanoribbons, VIVEK SHENOY, Brown University — We show that edge stresses introduce intrinsic ripples in free-standing graphene sheets even in the absence of any thermal effects. Compressive edge stresses along zigzag and armchair edges of the sheet cause out-of-plane warping to attain several degenerate mode shapes. Based on elastic plate theory, we identify scaling laws for the amplitude and penetration depth of edge ripples as a function of wavelength [1]. We also demonstrate that edge stresses can lead to twisting and scrolling of nanoribbons as seen in experiments. Our results underscore the importance of accounting for edge stresses in thermal theories and electronic structure calculations for free-standing graphene sheets. [1] V. B. Shenoy, C. D. Reddy, A. Ramasubramaniam and Y. W. Zhang, Phys. Rev. Lett. (in press)

1:15PM Q25.00009 Infrared spectroscopy of electronic bands in bilayer graphene1, ALEXEY KUZMENKO, ERIK VAN HEUMEN, DIRK VAN DER MARIEL, University of Geneva, PHILIPPE LERCH, Paul Scherrer Institute, Switzerland, PETER BLAKE, KONSTANTIN NOVOSELOV, ANDRE GEIM, University of Manchester — We present infrared spectra (0.11 eV) of electrostatically gated bilayer graphene as a function of doping and compare them with tight binding calculations. All major spectral features corresponding to the expected interband transitions are identified in the spectra: a strong peak due to transitions between parallel split-off bands and two onset-like features due to transitions between valence and conduction bands. A significant electron-hole asymmetry is observed.

1:27PM Q25.00010 Sharp Landau Levels in Scanning Tunneling Spectroscopy of Epitaxial Graphene on SiC(000 -1), DAVID MILLER, KEVIN KUBISTA, GREGORY RUTTER, MING RUAN, WALT DE HEER, PHILLIP FIRST, Georgia Institute of Technology, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST — Monolayer graphene has unique electronic properties stemming from a low-energy band structure that is linear, with chiral Dirac quasiparticles. In a magnetic field, the Landau level (LL) energies for graphene vary proportional to $\sqrt{nB}$, where $n$ is the LL index. Conversely, Bernal-stacked bilayer graphene and graphite have parabolic dispersion at low energies, resulting in $E_n \propto B^n$. In this talk we measure the LL spectrum of the top graphene layer directly via scanning tunneling spectroscopy (STS) at a 4.3 K. We show that for $n \approx 10$-layer epitaxial graphene grown on SiC(000 -1), the spectrum exhibits very sharp peaks (including a strong $n=0$ peak) spaced as $E_n \propto \sqrt{nB}$. This spectrum indicates that the rotational stacking in multilayer epitaxial graphene effectively decouples the layers, producing single-layer graphane behavior. Work supported in part by NSF, NRI-INDEX, and the W. M. Keck Foundation.

1:39PM Q25.00011 Electronic structures of single- and multi-layer epitaxial graphene on SiC (0001), SEUNGCHUL KIM, JISOON IHM, Department of Physics and Astronomy, Seoul National University, YOUNG-WOO SON, Korea Institute for Advanced Study — The electronic structures of single- and multi-layered epitaxial graphene on silicon carbide (0001) surface are studied theoretically. To calculate energy bands of the systems, we construct the simple Hamiltonian with tight-binding approximations. We confirm that the present simple model do not vary proportional to $n$. This spectrum indicates that the rotational stacking in multilayer epitaxial graphene effectively decouples the layers, producing single-layer graphane behavior. We extend the model up to four epitaxial graphene layers to explain various interesting experimental findings. The roles of the coupling between graphene bilayers and the buffer layer, and their large scale reconstructions to the electronic structures are also investigated. [1] S. Kim, J. Ihm, H. J. Choi, Y.-W. Son, Phys. Rev. Lett. 100, 176802 (2008).

1:51PM Q25.00012 G-band Phonon Symmetry Breaking of Graphene Monolayers, LAIN-JONG LI, YANG ZHAO, XIAOCHEN DONG, PENG CHEN, Nanyang Technological University — Aromatic molecules can effectively exfoliate graphite into graphene monolayers. And the resulting graphene monolayers sandwiched by the aromatic molecules exhibit pronounced G-band splitting, similar to that observed in rolled-up graphene sheet (single-walled carbon nanotubes). Raman measurements and the theoretical calculation based on force-constant model demonstrate that aromatic molecules are able to induce G-band splitting via breaking the symmetry of two in-plane longitudinal and transverse optical phonons at Gamma-point.

2:03PM Q25.00013 Edge states in a honeycomb lattice: effects of anisotropic hopping and mixed edges, ZI-XIANG HU, Zhejiang Institute of Modern Physics, Zhejiang University, China, HARI DAHAL, NIKOLAI SINITSYN, Los Alamos National Laboratory, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University, ALEXANDER BALATSKY, Los Alamos National Laboratory — We study the effects of anisotropic hopping and mixed edges on the edge states of graphene. The discussion of the edge states in graphene so far is focused on either zigzag or armchair edge with isotropic hopping. In this case the zigzag (arm chair) edge has enhanced (suppressed) local density of states at $E=0$ near the edge. In practice electrons in graphene can have anisotropic hopping. The lattice can have mixed (zigzag and arm chair) edges. Hence we study the effects of the anisotropic hopping and mixed edges on the edge states. We show that the mixed edges smear the enhanced local density of states at $E=0$ of the zigzag edge and, the anisotropic hopping enhanced the LDOS at $E=0$ in the armchair edge. Edge states in graphene can be studied using scanning tunneling microscopy (STM) experiments. We suggest that care must be taken while interpreting the STM data because the distinction between the zigzag and arm chair edge will be affected by the anisotropic electron hopping and the mixed edges.


11:15AM Q26.00001 Electron-electron interactions in graphene bilayers1, FAN ZHANG, HONGKI MIN, MARCO POLINI, ALLAN MACDONALD, DEPARTMENT OF PHYSICS, UNIVERSITY OF TEXAS AT AUSTIN COLLABORATION, NEST-CNR-INFN AND SCUOLA NORMALE SUPERIORE COLLABORATION — Electrons in condensed matter normally form Fermi-liquid states in which e-e interactions play an inessential role. A well known exception is the case of 1D electron systems in which the Fermi-surface consists of two points and divergences associated with low-energy particle-hole excitations abound when e-e interactions are described perturbatively. Corresponding divergences normally occur in systems with higher space dimensions when Fermi lines or surfaces satisfy idealized nesting conditions. Here we discuss the role of e-e interactions in 2D graphene bilayers which behave in many ways as if they were 1D because they have point-like Fermi surfaces which satisfy the nesting condition and have two-layer chirality and because their particle-hole energies have a quadratic dispersion which compensates for the difference between 1D and 2D phase spaces. We conclude, on the basis of a perturbative RG calculation, that interaction in neutral graphene bilayers drive the system into a spontaneously broken symmetry state with layer-pseudospin ferromagnetism.

1This work has been supported by the Welch Foundation and by the National Science Foundation under grant DMR-0606489.
11:27AM Q26.00002 Ferromagnetism in Graphene Stacks, DAGIM TILAHUN, ALLAN MACDONALD, The University of Texas at Austin — Because the density of states at the Fermi level of neutral graphene layers is proportional to external magnetic field, the ground state in strong fields is expected to have a broken symmetry - most likely ferromagnetism. In systems with stacked graphene layers this tendency competes with inter-layer hopping which favors paramagnetic ground states or perhaps other types of broken symmetries. We present a criterion for the stability of the ferromagnetic state and discuss its application to single-layer graphene, to weakly coupled epitaxial graphene layers on SiC or other substrates, and to bulk graphite. We use the Slonczewski-Weiss-McClure model to explain why the dominant inter-layer hopping process in Bernal (AB) stacked graphite does not compete with ferromagnetism.

11:39AM Q26.00003 Theory of inter-edge superexchange in zigzag edge magnetism, JEIL JUNG, Department of Physics, University of Texas at Austin, USA, TAMÍ PÉREZ-BARNEA, Physics Department, California Institute of Technology, USA, ALLAN MACDONALD, Department of Physics, University of Texas at Austin, USA — A graphene nanoribbon with zigzag edges has a gapped magnetic ground state with an antiferromagnetic inter-edge superexchange interaction. We present a theory based on the asymptotic properties of the Dirac-model ribbon wavefunction which predicts $W^{-2}$ and $W^{-1}$ ribbon-width dependences for the superexchange interaction strength and the gap respectively. Unlike in conventional superexchange we find that both the kinetic and exchange energy contributions favor the antiferromagnetic inter-edge coupling with a dominant role of exchange several times larger in magnitude than the kinetic energy contribution.

11:51AM Q26.00004 Numerical study on electron-electron interaction and ferromagnetic fluctuation in graphene, TIANXING MA, Max Planck Institute for the Physics of Complex Systems, Nöthenstr. 38, D-01187 Dresden, Germany, FEIMING HU, Department of Physics and the Institute of Theoretical Physics, the Chinese University of Hong Kong, ZHONGBING HUANG, Faculty of Physics and Electronic Technology, Hubei University, Wuhan 430062, People’s Republic of China, HAI-QING LIN, Department of Physics and the Institute of Theoretical Physics, the Chinese University of Hong Kong — Within the Hubbard model on a honeycomb lattice, we investigate the effect of electron-electron interactions and ferromagnetic fluctuations in graphene numerically. We find that the system in the filling region $\langle n \rangle > 1.60-1.90$ shows a short-ranged ferromagnetic correlation, and the on-site Coulomb interaction tends to strengthen ferromagnetic fluctuation slightly. Furthermore, the ferromagnetic fluctuation is strengthened markedly as the next-nearest-neighbor hoping energy increases, which indicate that the next-nearest-neighbor hoping term plays an important role in graphene since it breaks the particle-hole-symmetry.

12:03PM Q26.00005 Gate-induced interlayer asymmetry in ABA-stacked trilayer graphene, EDWARD MCCANN, Lancaster University, MIKITO KOSHINO, Tokyo Institute of Technology, Japan — We model the electronic band structure and conductivity of ABA-stacked trilayer graphene in the presence of external gates, self-consistently calculating the electric potential of the three layers. We show that a gate field perpendicular to the layers breaks mirror reflection symmetry with respect to the central layer, leading to hybridization of the linear and parabolic low-energy bands. For large gate fields, we derive an effective two-component Hamiltonian describing chiral electrons in two low-energy bands that exhibit an anti-crossing with a small hybridization gap. The magnitude of the gap is largely independent of the gate field, but the momentum at the anti-crossing and the typical band velocity both increase with it. Using the self-consistent Born approximation, we find that the density of states and the minimal conductivity in the presence of disorder generally increase as the gate field increases, in sharp contrast with bilayer graphene.

12:15PM Q26.00006 Aharonov-Bohm-like scattering, localization, and novel electronic states in hydrogenated graphene, ANDREY SHYTTOV, Utah University, DMITRY ABANIN, Princeton University, LEONID LEVITOV, Massachusetts Institute of Technology — Metallic nature of transport in graphene, which is fairly robust with respect to varying amounts of disorder, changes in an unexpected way when vacancies are introduced in this material. At low energies, near the Dirac point, electron scattering on vacancies mimics scattering on Aharonov-Bohm solenoids carrying unit flux. This type of scattering results in a very narrow band of states at the Dirac point with properties resembling those of zeroth Landau level, which is positioned in the middle of a (pseudo)gap created by vacancies and resembling the cyclotron gap around zeroth Landau level. The fictitious magnetic field describing vacancies has opposite signs for the valleys K and K'. As a result of this, an externally applied magnetic field has opposite effects in the two valleys, suppressing (reinforcing) the gap in the K (K') valley. We show that this picture is in agreement with the behavior observed in a recent study [1] of electronic properties of graphene, which can be transformed from metallic state to insulating state by hydrogenation. [1] D. C. Elias, R. R. Nair, T. M. G. Mohiuddin, S. V. Morozov, P. Blake, M. P. Halsall, A. C. Ferrari, D. W. Boukhvalov, M. I. Katsnelson, A. K. Geim, K. S. Novoselov, arXiv:0810.4706

12:27PM Q26.00007 Rashba spin-orbit interactions in zigzag graphene nano-ribbons, MAHDI ZAREA, Ohio University, NANCY SANDLER, Ohio University — The crystalline structure of graphene can be described in terms of a pseudo-spin degree of freedom and spinor wavefunctions. This characteristic has important physical consequences not observed in normal semiconductors. For zigzag ribbons, for instance, this translates into the existence of localized chiral edge states, with momentum coupled to pseudo-spin. In the presence of Rashba spin-orbit interactions (RSOI), this special feature makes the material a good candidate to produce localized spin polarized currents. To address this issue we investigated the role of the RSOI on the band-structure and wavefunctions of an infinite graphene plane and a zigzag nano-ribbon. We present analytic and numerical results showing that the spin profile along the edge is state-dependent. We compare these results with the profiles obtained in the presence of the intrinsic spin-orbit interaction [1]. We show that the RSOI can create average localized spin polarized currents along the edges of zigzag ribbons with appropriate applied voltages. [1] Zarea, M., Busser, C. and Sandler, N. PRL 101, 196804 (2008).

1Work supported by OU postdoctoral fellowship and OU-BNNT programs.

12:39PM Q26.00008 Plasma Instabilities in Graphene, BEN YU-KUANG HU, The University of Akron, ANTTI-PEKKKA JAUHO, Techn. Univ. of Denmark and Helsinki Institute of Technology — We discuss the possibility of the occurrence of plasma instabilities under non-equilibrium conditions in graphene. Specifically, we investigate the stability of the collective electronic modes in graphene with two counter-streaming distributions of carriers by studying the frequency-dependent dielectric function $\varepsilon(q, \omega)$ of the system. We find that the linear electronic dispersion of graphene results in instabilities that are qualitatively different from the standard two-stream instabilities for classical plasmas and parabolic-band systems.

12:51PM Q26.00009 Is suspended graphene an insulator?, JOAQUIN DRUT, The Ohio State University, TIMO LAHDE, University of Washington — Graphene at low energies resembles massless quantum electrodynamics in a strongly coupled regime, away from the usual perturbative region where the fine structure constant is $\alpha \sim 1/137$. Indeed, a single sheet of graphene in vacuum presents $\alpha \sim 1$. At such strong couplings the U(4) chiral symmetry of graphene can spontaneously break, inducing a gap in the quasiparticle spectrum. The question of whether chiral symmetry is broken represents a computational challenge that lies outside the domain of analytic techniques. In this talk, we will present the results of the first Monte Carlo simulation of the low-energy effective theory of graphene in vacuum (see abstract by T. A. Lähde). We have computed the chiral condensate, which is the order parameter for the insulating charge density wave state, as a function of $\alpha$, and found a chiral phase transition that is compatible with suspended graphene being in the gaped phase.
1:03PM Q26.00010 Many-body effects in neutral graphene bilayers . CSABA TOKE, Lancaster University, VLADIMIR I. FALKO, Lancaster University — A graphene bilayer is studied within the Hartree-Fock approximation in the tight-binding model. The exchange self-energy is studied systematically in an momentum expansion. Up to first order in the coupling constant (the effective fine structure constant) and to first order of the nonperpendicular hopping parameter we find that, for zero magnetic field, the exchange interaction with the valence band contributes with a logarithmically divergent correction to the Fermi velocity, the perpendicular inter-layer hopping, and the tringular warping. The effective mass renormalization in the two-band effective Hamiltonian is studied. For a strong perpendicular magnetic field the exciton dispersions are calculated.

1:15PM Q26.00011 Berry phase and the role of trigonal warping in graphene systems . IVAN STANIC, KARYN LE HUR, Yale University — In general Dirac fermions exhibit a Berry phase of $\pi$ whereas non-relativistic free-like particles have a Berry phase of $2\pi$. The two cases have been reported, both theoretically and experimentally, in single-layer and bi-layer graphene respectively. On the other hand, if one considers, for example, bi-layer graphene in more detail, its band structure shows both the Dirac-type, coming from the trigonal warping, and the parabolic, non-relativistic aspect in different energy regimes. This gives an unprecedented opportunity to investigate the crossover between non-relativistic and Dirac fermions in a Berry phase formulation. Here, we propose a scattering type-experiment (reflecting the Berry phase) to demonstrate this crossover. We present our theoretical results on scattering cross-sections taking into account the trigonal warping term, which confirm the jump in the Berry phase from $\pi$ to $2\pi$ as the energy of the incoming electrons is increased. This jump in the Berry phase can be understood from a general theorem relating the Berry phase and the band structure of a material.

1:27PM Q26.00012 Trigonal Band Structure and Time-Reversal Invariance in Graphene . ROLAND WINKLER, Northern Illinois University, ULRICH ZUELICKE, Massey University — We present a symmetry analysis of the trigonal band structure in graphene. While the energy spectrum near the Fermi edge equals the spectrum of massless Dirac fermions, the transformational properties of the underlying basis functions are qualitatively different. Using group theory we develop an invariant expansion of the Hamiltonian for the electron states near the $K$ points of the graphene Brillouin zone. We find that the $k$-linear dispersion near the band edge arises as an unusual consequence of time-reversal invariance. We suggest to divide the electronic properties of graphene into two categories, those that depend and those that do not depend on the transformational properties of the Bloch functions at $K$. See arXiv:0807.4204.

1:39PM Q26.00013 Two dimensional massless Dirac fermions with Coulomb interaction and random gauge potential . SEN HOU, OSKAR VAFEK, Florida State University — We present a numerical study of the two dimensional massless Dirac fermions of monolayer graphene with long-range Coulomb interaction and random gauge potential. The Coulomb interaction renormalizes logarithmically the electron velocity at low energies, leading to a decrease in the density of states. While the density of states is enhanced by the random gauge potential, and has a power-law dependence in low energies, $\rho(E) \sim E^{-1+2/z}$ with $z = 1 + \sqrt{3} \Delta / \pi$, where $\Delta$ measures the disorder strength. The combined effect of interaction and disorder gives rise to a line of fixed points where both the interaction and disorder are finite, and the low-energy density of states is exactly linear. Results are consistent with previous renormalization group argument.

2:03PM Q26.00015 Transport of massless Dirac fermions in graphene layers in presence of electromagnetic potential barriers . SANKALPA GHOSH, MANISH SHARMA, Indian Institute of Technology Delhi — We study the transport of massless Dirac fermions in Graphene layers through electromagnetic potential barriers. The barriers consist of periodically arranged delta function-electromagnetic potential barriers, SANKALPA GHOSH, MANISH SHARMA, Indian Institute of Technology Delhi — We study the transport of massless Dirac fermions in graphene layers through electromagnetic potential barriers. The barriers consist of periodically arranged delta function-electromagnetic potential barriers.

2:11PM Q26.00016 Gap opening due to topological defects in graphene . RICARDO NUNES, JOICE ARAÚJO, HELIO CHACHAM, UFMG - Brazil — Stone-Wales defects (SWD = two adjacent pentagon-heptagon pairs) are common low-energy defects in carbon nanotubes. Previously, Crespi et al.[PRB, 53, 1996] have proposed a purely-carbon covalent metal sheet called “pentaheptite,” consisting entirely of SWDs, with a relatively low formation energy of 0.32 eV/atom, with respect to graphene. In this work, we consider three different families of periodic carbon sheets containing topological defects (TDs = pentagons and heptagons). The families differ by the density of TDs in a seed structure. In each family, we generate periodic structures in which isolated pentagons and heptagons are surrounded only by hexagons. By means of ab initio calculations, we propose that, depending on the density and distribution of TDs, these carbon sheets may behave as a semiconductor, a metal or a semimetal. In the range of TD concentrations we examine, the sheets are stable in a planar form, but, allowing for the corrugation generated by the curvature fields associated with the isolated TDs, leads to lower formation energies and to either a reduction of the density of states or to gap opening at the Fermi level. Formation energies can be very small: in particular, we obtain a semiconducting structure with a formation energy of only 92 meV/atom with respect to graphene.

3:29PM Q26.00017 Berry phase formulation of transport through Graphene, and the associated problems can be mapped on certain classes of optical problems. We discuss the related band structure and its effect on transport over a range of magnetic field strengths and barrier widths. We also discuss the typical experimental set up where related properties can be verified.

Wednesday, March 18, 2009 11:15AM - 2:15PM — Session Q27 GIMS: Focus Session: X-ray and Neutron Instruments and Sciences II 329

11:15AM Q27.00001 3D Mapping of Strain and Dislocation Gradients near Surfaces and Interfaces via Polychromatic Microdiffraction . ROZALIYA BARABASH, GENE ICE, Oak Ridge National Laboratory — The results of 3D polychromatic X-ray microbeam analysis (PXM) of strain and dislocation gradients are presented. Two examples are considered: (1) FIB machined nano-size trenches in thin GaN/InGaN multilayers; (2) natural nanosize Mo pillars in the NiAl matrix of the eutectic composite alloy. Position sensitive $d$-spacings were obtained from Laue patterns. The PXM results show that FIB induces structural changes and lattice rotations in the InGaN/GaN layer not only in the immediate trench region but in the surrounding area as well. For embedded nanosize Mo fibers, the measured elastic strain is consistent with the predicted thermal mismatch strain between the NiAl and Mo phases. However, when the NiAl matrix is etched back to expose Mo micro-pillars, the $d$-spacing increases to that of unconstrained Mo, indicating release of the compressive residual strain in the Mo fibers.

1Research is sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Science, U.S. Department of Energy.
11:27AM Q27.00002 Strain Fields in Zeolite Microcrystals by Coherent X-ray Diffraction1, HYUNJUNG KIM, Sogang University, WONSUK CHA, SANGHOON SONG, NAK CHEON JEONG, KYUNG BYUNG YOON, Sogang University, Korea, ROSS HARDER, Advanced Photon Source, ANL, IAN K. ROBINSON, , University College London, United Kingdom — We measured coherent X-ray diffraction (CXD) on zeolite microcrystals in order to get information on internal density distribution and to map deformation field of stress or strain during the fabrication process. The experiments were performed at the beamline 34-ID-C in Advanced Photon Source and employed monochromatic radiation with x-ray energy of 9 keV. The sample size was about \( \sim 2\mu \text{m} \). The diffraction patterns were obtained at (200) Bragg condition with unfocused beam. We inverted the diffraction patterns to obtain three dimensional images of the shapes and internal strain fields of zeolite microcrystals using phase retrieval algorithms of error reduction and hybrid input-output method. The internal density and strain distribution as a function of temperature will be discussed.

1This work was supported by Korea Science & Engineering Foundation and Seoul Research and Business Development Program (10816).

11:39AM Q27.00003 Silicon x-ray monochromator surfaces by independent oxidation and etching steps1, ALBERT MACRANDER, Advanced Photon Source, Argonne, KIMBERLEY MACARTHUR, EE Dept. Northern Illinois Univ., JOSEF MAJ, JIJN QIAN, APS, Argonne, DAN LINNEN, EE, NIU, RUBEN KHACHATRYAN, MICHAEL WIECZOREK, APS, Argonne, RAY CONLEY, NSLS II, Brookhaven, ALAN GENIS, EE, NIU — X-ray monochromators should ideally possess a surface that does not distort a diffracted beam. Beam distortions have been observed at the APS for rough surfaces. Mechanical polishing leaves sub-surface damage. The standard method to remove this damage is to wet etch Si crystals in a mixture of nitric acid and hydrofluoric acid. During the etch an oxide is produced and removed in the same acid bath. X-ray diffraction from a bulk reflection that is largely unaffected by strain can be obtained by this method. However, the smoothness is degraded to produce an orange-peel morphology. For the present study we carried out the oxidation and etching steps independently. By first growing an oxide layer in a furnace and subsequently etching away the oxide layer, we find that sub-surface damage can be removed and the surface quality can be improved over that found with only wet etching.

1Work supported by US DOE, Office of Science, Basic Energy Sciences under Contract No. DE-AC02-06CH11357

11:51AM Q27.00004 Observation of annealing of grains in high purity aluminum using High Energy X-ray Diffraction Microscopy , C.M. HEFFERAN, S.F. LI, Carnegie Mellon University, U. LIENERT, Argonne National Laboratory, R.M. SUTER, Carnegie Mellon University — High energy x-ray diffraction microscopy (HEDM) is capable of measuring volumes of polycrystal microstructure on a granular basis, producing spatial maps of crystallographic orientation covering ensembles of grains with micron resolution. A non-destructive experimental probe capable of observing the response of polycrystals to thermo-mechanical stimulus, HEDM establishes constraints on analytic materials models. HEDM uses high-brilliance, line focused synchrotron x-rays to image diffracted beams emanating from individual grains in a succession of planar sections. Area detector images of diffraction patterns are collected as the sample rotates normal to the beam plane. A forward modeling computer simulation adjusts local crystallographic orientations and compares simulated scattering to experimental images in order to optimize the match with observations. Three dimensional digital representations are generated from large numbers of reconstructed sections. Growth measurements on high purity polycrystalline aluminum have been conducted at the 1-ID beamline at the Advance Photon Source at Argonne National Laboratory and reconstructions have been obtained using the Pittsburgh Supercomputing Center. Both defect annealing and grain boundary motions have been observed and will be described.

12:03PM Q27.00005 Strain Analysis in 2D and 3D X-ray Microscopy1, J.Z. TISCHLER, B.C. LARSON, ORNL, WENJUN LIU, ANL, LYLE LEVINE, NIST — Spatially resolved strain distributions on the submicron length scale are important for materials problems such as deformation and phase separation, and in heterogeneous systems in general. High-energy 3DXRD techniques have been developed by RISO with a few micron 3D resolution for lightly deformed materials. However, submicron 3D spatial distributions of local strain in heavily deformed materials are often required, such as in for multiscale materials modeling. We have developed a scanning-monochromatic x-ray microbeam technique on sector-34 of the Advanced Photon Source to measure the Q-distribution from submicron volume elements in lightly and heavily deformed materials and in single, polycrystalline, or composite materials. By sorting the intensity from every pixel in an area detector during nested energy and differential aperture depth scans, Q-distributions are obtained for every spatially resolved volume element. We will present measurement examples and discuss the range of applications.

1ORNL research sponsored by DOE Office of Basic Energy Sciences, Div. of Materials Sciences & Engineering; XOR-UNI and APS are supported by DOE-BES.

12:15PM Q27.00006 Towards mapping of defected grains using high energy x-ray diffraction microscopy , SHIU FAI LI, C.M. HEFFERAN, Carnegie Mellon University, U. LIENERT, Argonne National Laboratory, R.M. SUTER, Carnegie Mellon University — High energy x-ray diffraction microscopy (HEDM), the use of focused high energy synchrotron x-ray radiation diffraction imaging, is becoming a promising technique for orientation mapping of polycrystalline material. The nondestructive nature of HEDM makes real-time observation of inter- and intra-grain dynamics possible. Collected HEDM data in the form of diffracted images on a high resolution 2D detector is analyzed by a Monte Carlo fitting algorithm using a forward modeling method, which simulates a set of detector images based from a specified orientation field. Since no specific assumptions are made regarding grain shapes and topologies, internal mosaic structures may be captured. The combination of nondestructive nature and intra-grain resolution makes it an ideal candidate for in situ studies of grain damage due to strain/stress treatment. A proof of concept has been demonstrated in observations of internal mosaic structures may be captured. The combination of nondestructive nature and intra-grain resolution makes it an ideal candidate for in situ studies of grain damage due to strain/stress treatment. A proof of concept has been demonstrated in observations of grain shapes and topologies. The nondestructive nature of HEDM makes real-time observation of inter- and intra-grain dynamics possible. The nondestructive nature of HEDM makes real-time observation of inter- and intra-grain dynamics possible.

12:27PM Q27.00007 A Holographic Iterative Algorithm for X-ray Microscopy1, DILING ZHU, Department of Applied Physics, Stanford University, BENNY WU, RAMON RICK, Department of Applied Physics, Stanford University, JOACHIM STÖHR, ANDREAS SCHERZ, Stanford Synchrotron Radiation Lightsource — In recent years X-ray Fourier transform holography has gained recognition as a high resolution microscopy technique. The phase information is encoded in the hologram which renders this a lessens approach as a true imaging technique by applying a simple inverse Fourier transform. In previous experiments the resolution was limited by imperfect knowledge of the reference and therefore was determined by the size of the reference. We report an alternative technique based on direct calculation of the encoded phase by recording multiple holograms. This phase information provides additional constraints to fully deconvolve the reference and the object using iterative phase retrieval algorithms. In numerical simulations we observe rapid convergence of this new reference-guided phase retrieval method which also shows high immunity against noise. We present two different experimental implementations and their results to demonstrate the feasibility of the concept.

1The experiments were carried at SSRL. Both SSRL and the conducted research are supported by the U. S. Department of Energy, Office of Basic Energy Sciences.
12:39PM Q27.00008 New Method for Inverting X-ray Holographs , YUHAO WANG, New Jersey Institute of Technology, JIANMING BAI, University of Tennessee, TREVOR A. TYSON, New Jersey Institute of Technology, PETER SIDDONS, GIANLUIGI DE GERONIMO, Brookhaven National Laboratory — The matrix solving method is a new class of methods to be applied to inverting an x-ray hologram for obtaining real space structures. The method is shown to provide better resolution and more flexibility than Fourier transform methods. Simulations suggest that non-direct scheme non-indirect scheme x-ray fluorescence hologram, measured with both fixed light source and fixed detector can be inverted with the matrix solving method. Applying pre-determined non negative restrictions can improve the spatial resolution and approach the wavelength of the measuring x-rays. Experimental details and methods for measuring x-ray florescence holography with the matrix solving inversion is discussed. This work is supported by NSF DMR grant MRI-0722730.

12:51PM Q27.00009 Growth and characterization of high k ZrO$_2$ on Ge (100) , ABDUL RUMAIZ, GABRIELLA CARINI, PETER SIDDONS, NSLS, Brookhaven National Laboratory, JOSEPH WOICIK, NIST, PAVEL REHAK, Brookhaven National Laboratory — The higher mobility of carriers combined with a low effective mass in Ge as compared to Si has generated a lot of interest in Ge based devices. This is particularly so in X-ray radiation detectors where Si based detectors become transparent at higher energy. The challenge in realizing a Ge based detector is having a robust barrier oxide. GeO$_2$ is the candidate oxide of choice for Ge. We have grown high k ZrO$_2$ on Ge (100) using direct metal sputtering followed by UV oxidation [1]. High energy X-ray photoelectron spectroscopy (XPS) was performed to study the oxidation state of ZrO2 as well as the interface with Ge. A simple structure with Ge/GeO$_2$/ZrO$_2$ (25 nm)/Al (200 nm) was created. A significant hysteresis was observed in the capacitance-voltage measurement which is indicative of some interface states [2]. The effect of the intermediate layer between ZrO2 and Ge on the interface states will be addressed. Valence band measurement done using high energy XPS will be discussed. [1] C. O. Chui, S. Ramanathan, B. B. Triplett, P. C. McIntrye and K. C. Sarawat, IEEE Electron Dev. Lett. 28, 473 (2002) [2] H. Kim, C.O. Chui, K. C. Sarawat and P.C. McIntrye, Appl. Phys. Lett. 83, 2647 (2003)

1:03PM Q27.00010 High-field pulsed magnet instruments for x-ray studies of materials at the Advanced Photon Source , ZAHIRUL ISLAM, Argone National Laboratory (ANL), J.P.C. RUFF, McMaster University, Y. MATSUDA, ISSP, University of Tokyo, Z. QU, Tulane University, H. NOJIRI, Tohoku University, B.D. GAULIN, McMaster University, S. YOSHII, Tohoku University, Z. MAO, Tulane University, J.C. LANG, ANL — High-field pulsed magnets are not the solution to x-ray studies of all problems requiring high magnetic fields, but, they are the only option to many. We present a very high-field pulsed magnet system for x-ray studies of materials at the Advanced Photon Source (APS). The high-field instruments for x-ray studies are unique in the United States. Currently, 30 Tesla split-coil and long-pulse solenoids are in use for scattering and spectroscopic experiments, respectively. The coils are made of CuAg wires. Pulsed fields (1-10 ms in duration) are generated using a configurable bipolar capacitor bank (40 kJ). For scattering studies split coils are mounted on the cold finger of a 10-20 minutes for peak fields in the range of 20-30 Tesla. Time-resolved scattering data are typically collected using a fast APD detector. Initial scattering studies of a geometrically frustrated magnet will be presented.

1:15PM Q27.00011 Longitudinal and Transverse Components in the X-ray Resonant Magnetic Reflectivity Experiment , J.-S. LEE, E. VESCOVO, C.-C. KAO, NSLS, J.-M. BEAUJOUR, A.D. KENT, NYU, H. JANG, J.-Y. KIM, J.-H. PARK, POSTECH, PLS COLLABORATION — X-Ray Resonant Magnetic Reflectivity (XMR) is a powerful tool: It allows to simultaneously probe the structural and the magnetic properties of complex multilayer structures. It is often advantageous to utilize circular polarized synchrotron radiation to obtain magnetic information. Unfortunately, in XRMR measurement using circular polarization, the transverse and longitudinal components are intrinsically mixed, making a proper vector-analysis of the magnetization usually impossible. In this work, we strive to overcome this restriction. In particular, we demonstrate how to effectively separate the transverse and longitudinal components in the scattering experiment using circular polarized light. This is accomplished by taking advantage of x-ray interference effects which fully suppress the longitudinal component at all angles where the magnetic asymmetry ratio is null. At these angles only the purely transverse component is therefore left in the data.

1:27PM Q27.00012 Monte-Carlo Resampling Analysis of Neutron and X-ray Reflection Data , F. HEINRICH, Carnegie Mellon University, Pittsburgh, PA, and NIST Center for Neutron Research, Gaithersburg, MD, P. SHEKHAR, Carnegie Mellon University, Pittsburgh, PA, P. KIENZLE, NIST Center for Neutron Research, Gaithersburg, MD, M. LOESCHE, Carnegie Mellon University, Pittsburgh, PA, and NIST Center for Neutron Research, Gaithersburg, MD — In most cases, reflectivity data analysis relies on the use of a structural model with reasonable constraints. Commonly, parameter confidence intervals are estimated, and the choice of the adequate model solely relies on the of the experimenter. We present the implementation of the Monte-Carlo resampling technique for X-ray and neutron reflectivity data analysis. We introduce an algorithm which samples the phase and the amplitude of the complex coefficient of the plane waves in the multiple scattering equations. We use this algorithm to reconstruct the phase of a dielectric mirror, and of a nematic liquid crystal cell. We also implement the same algorithm to perform a deconvolution of a rough surface. We then compare the results obtained with this algorithm with those obtained with direct solution of the matrix. The proposed algorithm is an efficient and easy to use method to get a first estimation of how the specular component of the reflection may depend on the membrane roughness. The algorithm has been implemented for X-ray and neutron data analysis.

1:39PM Q27.00013 Scattering Hybrid Metal-Single Crystal Slit for Small Angle X-ray Scattering and High Resolution X-ray Diffraction, YOULI LI, University of California Santa Barbara, ROY BECK, TUO HUANG, MYUNG CHUL CHOI, MORITO DIVINAGRACIA — A simple hybrid design has been developed to produce effectively scattering aperture slits for small angle x-ray scattering (SAXS) and high resolution x-ray diffraction. The hybrid slit consists of a single crystal (Si, Ge) edge bonded to a tapered high density metal base. The beam-defining single crystal tip is oriented at a large tilt angle with respect to the beam and far from any Bragg peak position, and hence should produce no slit scattering commonly associated with conventional metal slits. The scattering performance of the new slit design was confirmed by experiments conducted with laboratory x-ray sources as well as third generation synchrotron radiation. The new scattering slits have been successfully used for SAXS application, where it led to a greatly simplified Single Aperture SAXS design with dramatically increased intensity (3-fold observed) as well as improved low angle resolution compared to a conventional three-pinhole set up. Supported by NSF MRI Development grant DMR-0619171.

1:51PM Q27.00014 Resonant soft x-ray scattering from Cu valence modulations in oxygen ordered YBCO , DAVID HAWTHORN, University of Waterloo, K.M. SHEN, Cornell University, J. GECK, IFW-Dresden, D.C. PEETS, H. WADATI, RUIXING LIANG, D.A. BOWN, W.N. HARDY, G.A. SAWATZKY, University of British Columbia, J. OKAMOTO, D.J. HUANG, H.-J. LIN, NSRRC, Taiwan, JONATHAN DENLININGER, Lawrence Berkeley National Laboratory — Recently resonant elastic soft x-ray scattering (RSXS) has emerged as a powerful new tool to study electronic ordering in materials like cuprates and manganites. The power of this technique is to combine x-ray scattering, which is sensitive to spatial order, with x-ray spectroscopy, which is sensitive to the valence, spin and orbital symmetry of specific atoms. This combination allows one to probe very directly and considerable detail a variety of exotic spin, charge, orbital or structural ordering phenomena. I will discuss the application of this technique to an important test case, oxygen ordering in YBCO. In this system we are able to accurately calculate the energy dependence of the scattering intensity, providing a basis for understanding the spectroscopy of more complex systems.
2:03PM Q27.00015 Phase Separation of Water/Glycerol Binary Mixtures Next to Lipid Monolayers – An X-ray and Neutron Reflectivity Study1, LUKA POCIVAVSEK, BRIAN LEAHY, MATI MERON, BINHUA LIN, The University of Chicago, JAREK MAJEWSKI, LANL, KA YEE LEE, The University of Chicago. We recently developed a general model for studying instabilities like wrinkling and folding in interfacial membranes on fluid substrates. The dominant length scales describing the instability are set by the elastic response of the membrane (primarily bending) and the “stiffness” of the substrate. These length scales, like the wrinkle wavelength and fold amplitude, are independent of the particular interfacial molecular interactions for micron thick membranes where typical system energies like the membrane bending stiffness are thousands of times larger than intermolecular potentials. However, as the membranes become thinner and thinner and eventually approach molecular membranes only a couple of nanometers thin, the chemical interaction between the membrane and the fluid substrate strongly influence the wrinkling and folding length scales. We present data for two such systems (a lipid monolayer and a gold nanoparticle layer) on different hydrogen bonding fluids and discuss possible mechanisms and modifications of our wrinkle-to-fold scaling laws to account for this new degree of freedom.

1Chicago MRSEC, UChicago MSTP, CARS, Lujan Center


11:15AM Q28.00001 Carbon Dioxide Capture in Microporous Metal-Organic Frameworks . JEFFREY R. LONG, University of California, Berkeley — Metal-organic frameworks represent a new class of materials exhibiting high internal surface areas, tunable pore dimensions, and tailorable surface functionality. Research in our laboratory has focused on the development of metal-organic frameworks with surfaces bearing open metal coordination sites for high-enthalpy hydrogen adsorption. Recently, we have initiated efforts to utilize such materials for the selective capture of CO2 from flue gas. Here, open metal coordination sites can deliver a high CO2 loading capacity at low pressures. However, additional criteria, such as water stability and the selective binding of CO2 over N2, must also be taken into consideration. Towards that end, we have targeted air- and water-stable frameworks bearing surfaces coated with amine groups. For example, the use of 1,3,5-benzenetristriazolato (BTri)3− as a bridging ligand has led to sodalite-type frameworks such as HCu[(CuCl)3(BTC)]3, possessing open Cu2+ coordination sites and exhibiting good chemical and thermal stability. Attachment of ethylenediamine to the Cu2+ sites within this structure generates a material that selectively binds small amounts of CO2 over N2. Details of the characterization of this and related materials will be presented.

11:51AM Q28.00002 Hydrogen storage in a metal-organic-framework structure from a nonempirical van der Waals density functional approach1, LINGZHU KONG, Rutgers, VALENTINO C. COOPER, Rutgers & ORNL, NOUR NIJEM, YVES J. CHABAL, UT Dallas, KUNHAO LI, JING LI, DAVID C. LANGRETH, Rutgers — Hydrogen adsorption in the metal-organic-framework structure Zn2(BDC)2(TED) (BDC=benzenedicarboxylate; TED=triethylendiamine) is studied using a van der Waals-density-functional approach. Two types of adsorption sites are located in the structure. The binding energies and the number of such sites are in good agreement with the values obtained from the experimental isotherms and isosteric heat of adsorption. The stretching mode frequency of the adsorbed H2 is calculated for various H–H bond orientations at the two positions. The frequency changes by approximately ~90 cm−1 for the strongest binding direction at each of the two points, which is consistent with the measured infrared absorption band measured at 4120 cm−1 at room temperature and high pressures (300-800 psi).

1Supported by grants DOE-DE-FG02-08ER46491. Work by V.R.C. supported by NSF-DMR-0456957 at Rutgers and by DOE at ORNL.

2M. Dion et al., PRL 92, 246401 (2004); T. Thonhauser et al., PRB 76, 125112 (2007).


12:03PM Q28.00003 Enhanced H2 adsorption in metal-organic frameworks with open metal sites: Binding mechanism and strong dependence on metal ions1, WEI ZHOU, HUI WU, NIST and Univ. of Maryland, TANNER YILDIRIM, NIST and University of Pennsylvania — Metal-organic frameworks (MOFs) with open metal sites exhibit much stronger H2 binding strength than classical MOFs, due to the direct interaction between H2 and the coordinately unsaturated metal ions. [1] Here we will present a systematic study of the H2 adsorption on a series of isostructural MOFs, M2(H2)2 with open metal sites M = Mg, Mn, Co, Ni, Zn. The experimental, initial isosteric heats of adsorption for H2 (Qst) of these MOFs range from 8.5 to 12.9 KJ/mol, with increasing Qst in the following order: Zn, Mn, Mg, Co, and Ni. [2] The H2 binding energies derived from first-principles calculations follow the same trend as the experimental observation on Qst, confirming the electrostatic Coulomb attraction between the H2 and the open metal sites being the major interaction. We also found a strong correlation between the metal ion radius, the M-H2 binding strength and the coordinately unsaturated metal ions. [1] J. Phys. Chem. C, 112, 8132 (2008). [2] J. Am. Chem. Soc., 130, 15268 (2008).

1Partially supported by DOE BES-DE-FG02-08ER46522 (TY).

12:15PM Q28.00004 Noncovalent hydrogen bonding in metal-organic structures . NORM M. TUBMAN2, JONATHAN L. DUBOIS, RANDOLPH Q. HOOD, SEBASTIEN HAMEL, ERIC R. SCHWEGLER, Lawrence Livermore National Laboratory — Transition metal sites in metal-organic frameworks and in doped carbon structures are actively being studied for their potential properties of molecular hydrogen. We present a study of prototypical metal-organic structures that can be used to bind molecular hydrogen non-covalently. Due to the well known limitations of current density functional theory based descriptions of non-covalent hydrogen bonding we have focused our efforts on a consistent many-body approach based on the fixed-node diffusion Monte Carlo method. Accurate studies of binding energies and the effects of multiple hydrogens in these structures are presented. Prepared by LLNL under Contract DE-AC52-07NA27344

2Additional affiliation: Northwestern University, Evanston IL 60208

12:27PM Q28.00005 Pd-assisted hydrogen spillover on graphene and carbonanotubes . SA LI, PURU JENA, Virginia Commonwealth University, VIRGINIA COMMONWÉALTH UNIVERSITY TEAM — Addition of a small amount of Pd precursors on carbon nanotubes has recently been found to substantially improve the hydrogen uptake. In spite of several attempts, a fundamental understanding of how the catalyst works has remained unattainable. Using first principles methods we have investigated hydrogen spillover on Pd-doped graphene and (8,8) carbon nanotube. Through molecular dynamics (MD) simulations, we found that each Pd can bind to three pairs of hydrogen molecules on graphene and only one pair of hydrogen molecule on (8,8) nanotube at 300K. This difference is attributed to the effect of curvature. The hydrogen molecules were found to dissociate and bind to carbon surface once the Pd atom is saturated with hydrogen. These results provide important new insight to understand hydrogen spillover on carbon based materials.
12:39PM Q28.00006 Calcium-Decorated Carbon Nanotubes for Hydrogen Storage1, HOONKYUNG LEE, University of California Berkeley, JISOON IHM, Seoul National University, MARVIN L. COHEN, STEVEN G. LOÜIE, University of California Berkeley — Using the first-principles pseudopotential density-functional method, we carry out a systematic search for high-capacity hydrogen storage media based on individually dispersed calcium atoms on carbon nanotubes (CNTs). We find that Ca clustering is suppressed on boron-doped and defective carbon nanotubes and that up to six H2 molecules can bind to a Ca atom with a binding energy of ~0.2 eV/H2. We show that Ca-decorated CNTs with a concentration of ~6 at. % B doping can reach the gravimetric capacity of ~5 wt % hydrogen storage. We also will discuss the binding mechanism of the H2 molecules.

1This research was supported by the NSF under Grant No. DMR07-05941 and the U.S. DOE under Contract No. DE-AC02-05CH11231. Computation resource is supported by NERSC and NERAC.

12:51PM Q28.00007 Theoretical study of hydrogen storage in Ca-coated fullerenes, QIAN SUN, Peking University and Virginia Commonwealth University, QIAN WANG, Virginia Commonwealth University, YOSHI KAWAOE, Tohoku University, PURU JENA, Virginia Commonwealth University — First principles calculations based on gradient corrected density functional theory and molecular dynamics simulations of Ca decorated fullerene yield some novel results: (1) C60 fullerene decorated with 32 Ca atoms on each of its 20 hexagonal and 12 pentagonal faces is extremely stable. Unlike transition metal atoms that tend to cluster on a fullerene surface, Ca atoms remain isolated even at high temperatures. (2) C60Ca32 can absorb up to 62 H2 molecules in two layers. The first 30 H2 molecules dissociate and bind atomically on the 60 triangular faces of the fullerene with an average binding energy of 0.45 eV/H2, while the remaining 32 H2 molecules bond on the second layer quasi-molecularly with an average binding energy of 0.11 eV/H2. These binding energies are ideal for Ca coated C60 to operate as a hydrogen storage material at near ambient temperatures with fast kinetics. (3) The gravimetric density of this hydrogen storage material can reach 5.8 wt %. Simple model calculations show that this density is the limiting value for higher fullerenes.

1:03PM Q28.00008 Rotor in a Cage: Infrared Spectroscopy of an Endohedral Hydrogen-Fullerene Complex1, TOOMAS RÕOM, MIN GE, D. HÜVONEN, U. NAGEL, NICPB, Akademia tee 23, 12618 Tallinn, Estonia, S. MAMONE, A. DANIOUGNY, F. CUIDA, M. C. GROSSEL, M. CARRAVETTA, M. H. LEVITT, School of Chemistry, Southampton University, Southampton SO17 1BJ, UK, Y. MURATA, K. KOMATSU, Institute for Chemical Research, Kyoto University, Kyoto 611-0011, Japan — We report the observation of quantized translational and rotational motion of molecular hydrogen inside the cages of C60. Narrow infrared absorption lines at the temperature of 6 K correspond to vibrational excitations in combination with translational and rotational excitations and show well-resolved splittings due to the coupling between translational and rotational modes of the endohedral H2 molecule. A theoretical model shows that H2 inside C60 is a three-dimensional quantum rotor moving in a nearly spherical potential. The theory provides both the frequencies and the intensities of the observed infrared transitions. Good agreement with the experimental results is obtained by fitting a small number of empirical parameters to describe the confined potential, as well as the ortho to para ratio at 6 K and at elevated temperatures [S. Mamone, et al., arXiv:0807.1589v2].

1The support by the EstSF grants 6138 and 7011, the EPSRC, and the University Research Fellowship (Royal Society) is acknowledged.

1:15PM Q28.00009 Hydrogen storage in charge compensated organic molecular crystals, MINA YOON, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany and Oak Ridge National Laboratory, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — We propose charge compensated organic molecular crystals as a promising class of materials for hydrogen storage. Using quantum mechanical first-principles calculations based on numerical atom-centered orbitals as all-electron basis functions [1] we study the basic structural properties of molecular crystals consisting of parallel sheets of cations and anions (such as DMPH and TCNQ) stacked alternatingly. The long range dispersion interactions between the cations and anions, which are important for the stability of the crystals, were studied and compared using various DFT xc functionals, semi-empirical approach [2], and Møller-Plesset perturbation theory. The molecular configuration causes accumulation of electrons at acceptors and depletion at donors, which results in finite dipolar fields. Our study indicates that these fields make it possible to use charge compensated organic molecular crystals for hydrogen storage.

[1] V. Blum et al., FH ab initio molecular simulations (FH-aims) project.

1:27PM Q28.00010 Mg-doped GaN nanostructures: Energetics, magnetism and H2 adsorption, QIAN WANG, Virginia Commonwealth University, QIAN SUN, Peking University and Virginia Commonwealth University, PURU JENA, Virginia Commonwealth University — It has been shown that p-type GaN can greatly improve the performance of GaN-based devices. Mg is a suitable candidate dopant for p-type GaN. Since the ionic radius of Mg is comparable with that of Ga, Mg doping can be expected to eliminate self-compensation effects. Thus, synthesis of Mg-doped p-type GaN for fabrication of optoelectronic devices has been hotly pursued. Using density functional theory and generalized gradient approximation for exchange and correlation potential we show that Mg doped GaN nanocage and nanotube can be magnetic with Mg contributed spins distributed over the neighboring N sites. Mg atoms show no tendency for clustering and due to the positive charge residing on them; they can trap hydrogen in molecular form via the charge polarization mechanism. The binding energies of hydrogen lie in the range of 0.1–0.2 eV/H2 which are ideal for storage applications under ambient thermodynamic conditions.

1:39PM Q28.00011 The USDOE Hydrogen Program: Status and Performance Gaps of On-board Hydrogen Storage Technologies, GRACE ORDAZ, MONTEREY GARDINER, CAROLE READ, U.S. Dept. of Energy, NED STETSON, U.S. Dept. of Energy — The USDOE Hydrogen Program’s mission is to reduce oil use and carbon emissions in the US transportation sector and to enable clean, reliable energy for stationary and portable power generation. The requirements for vehicular hydrogen storage continue to be one of the most technically challenging barriers to the widespread commercialization of hydrogen fueled vehicles. The DOE applied hydrogen storage activity focuses primarily on the research and development of low-pressure, materials-based technologies to allow for a North American market driving range of more than 300 miles (500 km) while meeting packaging, cost, safety, and performance requirements to be competitive with current vehicles. This presentation summarizes the status, recent accomplishments and current performance gaps of hydrogen storage technologies primarily for transportation applications. Materials projects are focused in three main areas: metal hydrides, chemical hydrogen storage materials, and hydrogen sorbents. A new effort is the Hydrogen Storage Engineering Center of Excellence which will provide a coordinated approach to the engineering research and development of on-board storage and refueling systems. The presentation will especially highlight topics emphasized in the session theme.

Wednesday, March 18, 2009 11:15AM - 2:03PM –
Session Q29 DMP GMAG: Focus Session: Ordering in Complex Oxides 333
the successful induction of crystal chirality in a noncentrosymmetric canted antiferromagnet, CuB

11:15AM Q29.00001 Orbitals, reduced dimensionality and spin gaps in correlated oxides

11:51AM Q29.00002 Phase transitions and magnetostructural coupling in ZnCr2O4 from first principles

12:03PM Q29.00003 Charge-ordering in Magnetite studied by Magnetic Compton scattering

12:15PM Q29.00004 First-principles determined charge and orbital interactions in Fe3O4

12:27PM Q29.00005 Magnetic control of crystal chirality and gigantic magneto-chiral effect in CuB2O4

12:39PM Q29.00006 Proposed Orbital Ordering in MnV2O4 from First-principles Calculations

2. V. N. Glazkov et al., http://arxiv.org/abs/0807.0546

3. The authors acknowledge support of MPG-India partnergroup program for this work.
Kagome compounds, AMBESH DIXIT, C. SUDAKAR, Department of Physics and Astronomy, Wayne State University, N. ROGADO, DuPont, E. GROSON, Rice University, R.J. CAVA, Princeton University, A.P. RAMIREZ, LGS Innovations, GAVIN LAIVES, Department of Physics and Astronomy, Wayne State University — The transition metal vanadate oxides having a staircase Kagome lattice structure exhibit rich magnetic phase diagrams, which arise from the complex geometry of these materials. Among these compounds, Ni$_3$V$_2$O$_6$ is particularly widely studied, as it develops simultaneous ferroelectric and incommensurate magnetic ordering at a single phase transition. In order to investigate the low frequency spin dynamics in these layered materials, we have probed the ac magnetic properties in these systems. We find that the Cu, Co, and Mn systems display strong magnetic relaxation in a spin ordered phase, with activation energies on the order of hundreds of Kelvin. We discuss these results in the context of spin-glass behaviour and domain wall motion.

1:03PM Q29.00008 Effect of Zn doping on the phase transition temperatures of Ni$_3$V$_2$O$_6$, AKILA KUMARASIRI, PARASHU KHAREL, AMBESH DIXIT, GAVIN LAIVES, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48221 — There is a considerable interest in understanding the nature of magnetic phase transition in geometrically frustrated materials. Ni$_3$V$_2$O$_6$ is one such system, with spin-1 Ni$^{2+}$ ions forming a layered buckled Kagome structure. We have studied the effects of doping spin-0 Zn ions on the magnetic phase transitions of powder Ni$_{1-x}$Zn$_x$V$_2$O$_6$ using dielectric and heat capacity measurements. (Ni$_{1-x}$Zn$_x$)$_2$V$_2$O$_6$ powder samples were synthesized starting with a mixture of Ni, V and Zn metal organic solutions mixed at appropriate atomic ratio. XRD and Raman studies show that (Ni$_{1-x}$Zn$_x$)$_2$V$_2$O$_6$ powder samples annealed at 1000°C crystallize in Ni$_2$V$_2$O$_6$ structure without forming any secondary phases. We have observed from heat capacity measurements that the phase transitions $T_H$, $T_d$, and $T_C$ at 9.2K, 6.4K, and 3.9K expected for Ni$_2$V$_2$O$_6$ are present in our (Ni$_{1-x}$Zn$_x$)$_2$V$_2$O$_6$ samples up to a Zn concentration of 20%. The transition at 2.4 K was not clearly observed. All three transitions shift toward lower temperatures with an increase in Zn concentration. We will present the experimental results on the strong suppression of both $T_H$ and $T_d$ due to dilution of Ni$_2$V$_2$O$_6$ with non-magnetic Zn. We will present a quantitative comparison of this suppression with the 2D Ising and Heisenberg models.

1:15PM Q29.00009 Electrical control of direction of orbital stripes in charge-ordered state of single-layered manganite La$_{1/2}$Sr$_{3/2}$MnO$_4$, SHOTA KONNO, Department of Physics, Tohoku University, KOUJI TANIGUCHI, HAJIME SAGAYAMA, TAKA-HISA ARIMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University — Electrical control of the localized electron such as an electric-field induced metal-insulator transition in charge-orbital ordered (COO) state of perovskite-related manganese oxides has been intensively studied, since the large electroresistance effect in Pr$_{0.7}$Ca$_{0.3}$MnO$_3$ was reported[1]. Moreover, the formation of orbital stripes in the COO state gives rise to in-plane anisotropies in the electrical, magnetic, and optical properties. However, there are few reports on controlling anisotropic properties in the COO state. We report an electric-field effect on the in-plane anisotropy in the COO state of a layered manganite La$_{1/2}$Sr$_{3/2}$MnO$_4$. After applying an electric field, a 90-degree rotation of COO states has been observed by using a polarizing microscope. A drastic change of the volumes of two COO domains was confirmed by means of synchrotron X-ray diffraction. [1]A. Asamitsu et al., Nature 388, 50(1997).

1:27PM Q29.00010 Intersite charge transfer in the $A$-site-ordered LaCu$_8$Fe$_4$O$_{12}$ perovskite, YOUEEN LONG, Institute for Chemical Research, Kyoto University, NAOAKI HAYASHI, Graduate School of Human and Environmental Studies, Kyoto University, TAKASHI SAITO, MASAKI AZUMA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University — A novel transition metal oxide LaCu$_8$Fe$_4$O$_{12}$ was prepared at 10 GPa and 1400 K. It crystallizes an orthorhombic $I4/mmm$ structure. With an increase of the La content the materials became oxygen stoichiometric and a lowering of the crystal structure without forming any secondary phases. We have observed from heat capacity measurements that the phase transitions $T_H$ and $T_d$ at 9.2K, 6.4K, and 3.9K expected for Ni$_2$V$_2$O$_6$ are present in our (Ni$_{1-x}$Zn$_x$)$_2$V$_2$O$_6$ samples up to a Zn concentration of 20%. The transition at 2.4 K was not clearly observed. All three transitions shift toward lower temperatures with an increase in Zn concentration. We will present the experimental results on the strong suppression of both $T_H$ and $T_d$ due to dilution of Ni$_2$V$_2$O$_6$ with non-magnetic Zn. We will present a quantitative comparison of this suppression with the 2D Ising and Heisenberg models.

1:39PM Q29.00011 $A$-site Magnetism in Perovskites CaCu$_3$B$_2$O$_{12}$ ($B$ = Ge, Ti, Sn). TAKASHI SAITO, HIROSHI SHIRAKI, YUICHI SHIMAKAWA, Kyoto University, MASAICHIRO MIZUMAKI, Japan Synchrotron Radiation Research Institute — $A$-site-ordered perovskites CaCu$_3$Ge$_2$O$_{12}$ and CaCu$_3$Sn$_2$O$_{12}$, both isosstructural to antiferromagnetic CaCu$_3$Ti$_2$O$_{12}$, were found to be ferromagnets, which are very rare in cuprates. All of these materials may be called "$A$-site magnets", since they contain magnetic species only at the $A$-site of the perovskite ABO$_3$ structure. The ferromagneticism of CaCu$_3$B$_2$O$_{12}$ ($B$ = Ge, Sn) is attributed to the ferromagnetic direct exchange interaction, whereas antiferromagnetic superexchange interaction, due to the Cu(3d)-O(2p)-Ti(3d) orbital hybridization, is dominant in antiferromagnetic CaCu$_3$Ti$_2$O$_{12}$. The $A$-site magnetism is controlled by the electronic structure of the non-magnetic B-site. Solid solutions CaCu$_3$(Ge,Ti)$_2$O$_{12}$ and CaCu$_3$(Ti,Sn)$_2$O$_{12}$ display phase boundary between ferromagnetic and antiferromagnetic phases. [1] H. Shiraki, T. Saito, Y. Shimakawa et al., Phys. Rev. B, 76 (2007) 140403. [2] Y. Shimakawa, H. Shiraki and T. Saito, J. Phys. Soc. Jpn., 77 (2008) 113602.

1:51PM Q29.00012 Structure and properties of high-oxygen-pressure annealed Sr$_{1-x}$La$_x$Co$_{0.5}$Fe$_{0.5}$O$_{3-d}$ (0<x<0.5), S. REMSEN, K. SWIERCZEK, B. DABROWSKI, L. SUESCUN, S. KOLESNIK, Department of Physics, Northern Illinois University, DeKalb, IL and Materials Science Division, Argonne National Laboratory, Argonne, IL — Synthesis, oxygen content, structural, magnetic, and resistive properties will be discussed for the Sr$_{1-x}$La$_x$Co$_{0.5}$Fe$_{0.5}$O$_{3-d}$ perovskites. The x=0 sample shows oxygen-vacancy ordered Sr$_x$Co$_{0.5}$Fe$_{0.5}$O$_{2.75}$ tetragonal $I4/m$ structure. With an increase of the La content the materials become oxygen stoichiometric and a lowering of the crystal symmetry is observed from cubic Pm3m (x=0.1 and 0.2) to tetragonal $I4/mcm$ (x<0.3 and 0.4), and finally to monoclinic $I2/c$ (x>0.5). All samples show ferromagnetic ordering with the maximum Curie temperature near 290 K at x=0.2. Conductivity is enhanced and small negative magneto-resistance is observed below T$_C$. Transport measurements up to 1100°C show high conductivity that is affected by the varying oxygen content. Work at NIU was supported by the NSF (DMR-0706610) and at ANL by the U.S. DOE under contract No. DE-AC02-06CH11357.
11:15AM Q30.00001 Colossal ionic conductivity at ZrO$_2$:Y,O$_3$ /SrTiO$_3$ interfaces. JACOBO SANTAMARIA, J. GARCIA BARRIOCANAL, A. RIVERA CALZADA, Z. SEFRIOU, L. LEON, CFMC, Universidad Complutense de Madrid, Madrid 28040, Spain, E. IBORRA, Universidad Politécnica de Madrid. Madrid 28040, Spain., M. VARELA, S.J. PENNYCOOK, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — We describe the strong enhancement of the conductivity occurring at the interfaces of superlattices made by alternating 10 nm strontium titanate and 1 nm yttria stabilized zirconia (YSZ) layers. Conductivity is found to be as high as 0.014 S/cm at 357 K, with a substantial decrease of the activation energy for the dc ionic conductivity from 1.1 eV down to 0.64 eV. EELS analysis is consistent with a large number of interfacial oxygen vacancies and high disorder in the interface oxygen plane between YSZ and STO layers. Our results demonstrate that the design of suitable heterogeneous interfaces in epitaxial heterostructures might have important implications in the search of artificial nanostructures with high ionic conductivity. 


11:27AM Q30.00002 Origin of Colossal Ionic Conductivity in YSZ-STO Superlattices. TIMOTHY PENNYCOOK, MATTHEW BECK, KALMÁN VARGA, Vanderbilt University, MARIA VARELA, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — An eight order of magnitude increase in the ionic conductivity of yttria-stabilized zirconia (YSZ) has recently been demonstrated in YSZ/strontium titanate (STO) epitaxial heterostructures. YSZ is the preferred electrolyte for solid oxide fuel cells (SOFC), in which the ionic conductivity is the major factor limiting the energy conversion efficiency. A colossal increase in the ionic conductivity, therefore, goes along way towards increasing SOFC practicality by increasing efficiency overall and reducing the operating temperature necessary for efficient operation. We report density functional calculations that explain this colossal ionic conductivity as the result of a large 7% expansive in-plane strain of the YSZ. Molecular dynamics simulations of strained zirconia yield an activation energy for ionic conduction in agreement with experiment. Additionally, simulated annealing under these strain conditions reveals a new energy structure for which EELS simulations using the Z−1 approximation for the core hole are consistent with electron energy loss spectra from the thin, coherently strained, YSZ layers of the heterostructures. This work is supported by NSF grant DMR-0513048 and DOE Office of Basic Energy Sciences, Division of Materials Science and Engineering.

11:39AM Q30.00003 Non-uniform magnetization in LaAlO$_3$/SrTiO$_3$ superlattices. M.R. FITZSIMMONS, M. ZHERNIENKO, N. HENGARTNER, LANL, A. SHARONI, IVAN K. SCHULLER, UCSD, J. GARCIA-BARRIOCANAL, F.Y. BRUNO, J. SANTA-MARIA, U. Complutense Madrid, Spain — Recently, Brinkman et al., [Nature 6, 493 (2007)] reported magnetism induced at the interface between LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) inferred from transport measurements. They found the magnetization to be greatly enhanced at low temperatures (i.e., liquid He temperature) and by application of high (10+ T) fields. We report polarized neutron reflectometry measurements of the magnetization depth profile of two LAO/STO superlattices with the same number of bilayer repeats. For low temperatures and a field of 11 T, the intensities of the superlattice Bragg reflections for both samples exhibited a dependence upon neutron beam polarization. The spin dependence was much weaker at small field (and low temperature) and disappeared altogether at 11 T and 300 K. These observations demonstrate that the magnetization depth profile has the period of the LAO/STO superlattice. The neutron spin dependence was more pronounced for the sample with a thin LAO layer compared to one with a thick LAO layer, suggesting that the magnetism may be interfacial in origin.

11:51AM Q30.00004 How to make a cuprate Fermi surface out of a nickelate heterostructure, OLE KROGH ANDERSEN, Max-Planck Institute for Solid-State Research — Chaloupka and Khalilullin had the idea that it might be possible to make Ni$^{3+}$-based high-temperature superconductors by sandwiching NiO$_2$ layers between insulating layers through heterostructuring. Provided that spin-, charge-, and orbital ordering can be avoided, the confinement should make it possible to empty the Ni 3z$^2$−1 band, thus leaving the conduction electron in the Ni 2x$^2$ − y$^2$ band. Fabrication of such heterostructures are now being pursued in many laboratories. We have attempted to give theoretical guidance by performing calculations for numerous heterostructures using the local density-approximation in combination with static (LDA+U) and dynamical (LDA+DMFT) mean-field theory. We show how confinement together with electronic correlations can lead to a single-sheet Fermi surface with a shape like that of the cuprate superconductors with the highest transition temperatures; the Ni 3z$^2$−1 Wannier orbital now plays the role of the axial, Cu 4s-like orbital in the cuprates.

Since also strong antiferromagnetic fluctuations are present, the low-energy electronic and spin excitations should resemble those of high-temperature cuprate superconductors. Chemical modification of the insulating layers should make it possible to avoid spin-, charge-, and orbital ordering.

12:27PM Q30.00005 Interfaces in La$_2$NiO$_4$ − La$_2$CuO$_4$ superlattices, S. SMADICI, J. C. T. LEE, S. WANG, P. ABBAMONTE, University of Illinois at Urbana-Champaign, IL 61801, G. LOGVEÑOV, A. GOZAR, I. BOZOVIC, Brookhaven National Laboratory, Upton, NY 11973 — Ni substitution on Cu sites in underdoped La$_2$−xSr$_x$CuO$_4$ quickly restores Neel order. This was attributed to strong interaction between the Ni and doped holes. An open question was whether the additional Ni empty orbital or the different spin on Ni sites was at the origin of this strong interaction. We have addressed this problem with resonant soft x-ray scattering on the La$_2$NiO$_4$ − La$_2$CuO$_4$ heterostructure. La$_2$NiO$_4$ and La$_2$CuO$_4$ have close lattice structures and electronic configurations. However, the x-ray scattering contrast between superlattice layers is greatly enhanced at soft x-ray resonant energies. Here we report our measurements at the O K, Cu L, and Ni L edges of a model of the charge, orbital and spin structures in these superlattices will be presented with a special emphasis on the interface region. This work was supported by Grants. DE-FG02-06ER46285, DE-AC02-98CH10886, MA-509-MACA, DE-FG02-07ER46453 and DE-FG02-07ER46471.

12:39PM Q30.00006 Layer-by-layer growth by pulsed laser deposition in the unit-cell limit. M. KAREEV, University of Arkansas, S. PROSANDEEV, J. LIU, P. RYAN, J.W. FREELAND, J. CHAKHALIAN — Unlike conventional growth of complex oxide heterostructures, the ultimate unit cell limit imposes strict constrains for a multitude of parameters critical to layer-by-layer growth. Here we report on detailed analysis of far-from-equilibrium growth by interrupted pulsed laser deposition with application to RENiO$_3$/LaAlO$_3$ superlattices grown on a diverse set of substrates SrTiO$_3$, NdGaO$_3$, LSAT and LaAlO$_3$. A combination of in-situ high-pressure RHEED and AFM along with extensive data obtained from synchrotron based XRD and resonant XAS allows us critically assess the role of RHEED intensity oscillation and the effect of a polar/non-polar interface on the heteroepitaxial growth. The role of defects formed during the initial stages of growth is also addressed.

Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357. J.C. was supported by DOD-ARO under the Contract No. 0402-17291 and NSF Contract No. DMR-0747808.
12:51PM Q30.00007 Perfect dc conductance of a finite width Mott insulator sandwiched between metallic leads at zero temperature: a quantum emergent phenomenon in strongly correlated multilayers\(^1\), HAND ZENIA, JIM FREERICKS, Department of Physics, Georgetown University, Washington, DC 20057 USA, HULIKAL KRISHNAMURTHY, Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India, THOMAS PRUSCHKE, Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — Self-consistent inhomogeneous DMFT calculations as well as analytical investigations of the electronic structure of a multilayered device are presented. The device consists of two semi-infinite leads of a ballistic metal that sandwich an interacting barrier. The interactions in the barrier are described by the Hubbard model with the whole system particle-hole symmetric. We find that for a finite barrier no matter how strong the interaction, the system becomes a Fermi liquid with a perfect metallic conductivity at low enough temperature. We argue that at zero temperature and frequency the Luttinger theorem holds and that the system has a well defined Fermi surface. The perfect conductive state may be extremely fragile to finite temperature, finite driving electric fields, finite driving frequencies, or disorder, so it will often be difficult to see experimentally. We will discuss possible experimental realizations of the phenomena

\(^1\)National Science Foundation

1:03PM Q30.00008 Strongly Interacting Electrons at the Oxide Interfaces\(^1\), JACQUES CHAKHALIAN, University of Arkansas — Utilizing the recent advances in complex oxide synthesis, one can now combine materials with antagonistic order parameters to create new compounds in the form of heterostructures often with properties not attainable in the bulk\(^1\). Broken symmetries, strain, and modified local environment at the interface provide a unique route to manipulate the subtle energy balance in correlated materials with promise to create novel material phases and quantum states. Here we report on how the interface can be used to alter electronic, magnetic and orbital structure of multilayers composed of late transition metal oxides with specific examples from cuprates, manganites and nickelates. We will discuss the underlying challenges in growth of ultra-thin layers of complex oxides and illustrate the ways synchrotron based resonant x-ray spectroscopies and resonant x-ray diffraction can be used to probe bulk vs. interface properties to gain unique insight into the underlying physics. J. Chakhalian et al, Science, v. 314, 1114, (2007).

\(^1\)This work supported by DOE Contract No DE-AC02-06CH11357. The projects are supported by DOD-ARO under the Contract No. DE-AC02-06CH11357. The projects are supported by DOD-ARO under the Contract No. DE-AC02-06CH11357.

1:39PM Q30.00009 X-ray standing wave photoemission from multilayer nanostructures\(^1\), C. PAPP, B. BALKE, LBNL, C. SAKAI, S. UEDA, H. YOSHIKAWA, Y. YAMASHITA, S. L. HE, K. KOBAYASHI, SPRing 8, G. CONTI, Applied Materials, D. BUEGLER, C. SCHNEIDER, Juelich Research Center, C. S. FADLEY, UC Davis/LBNL, S. DOERING, U. BERGES, C. WESTPHAL, TU Dortmund — We have used soft and hard x-ray standing wave excitation of photoelectrons to study buried layers and interfaces in multilayer nanostructures. The samples were grown on synthetic multilayer mirrors, and the x-ray incidence was tuned to 1\(^st\) order Bragg reflection. Scanning angle, photon energy, or distance along a wedge profile in the sample permits scanning the resultant standing wave field through nm-scale structures and analyzing the depth distribution of their chemical, electronic, magnetic, and structural properties. Using harder x-ray excitation permits via the higher kinetic energy of the electrons studying those properties at greater depths. The systems discussed will be two related to magnetic tunnel junctions (magnesium oxide/iron and STO/LSMO), and one related to integrated circuit production (titanium nitride on silicon).

\(^1\)This work supported by DOE Contract No DE-AC02-06CH11231 and the Humboldt Foundation.

1:51PM Q30.00010 Competing anisotropies and complex magnetism in SrRuO\(_3\)/SrMnO\(_3\) superlattices\(^1\), OMAR CHMAISSEM, Y. CHOI, Y.C. TSENG, D. HASKEL, D.E. BROWN, S. KOLESNIK, D. DANAHER — Using element-specific x-ray resonance techniques, we have investigated the interfacial magnetic coupling in SrRuO\(_3\)/SrMnO\(_3\) superlattices. A strong out-of-plane SRO anisotropy coupled with AFM Ru-Mn interactions result in a canted Mn structure with a significant induced net Mn moment that reduces to zero under a strong magnetic field. At \(T > T_{CSR/O}\), the SRO anisotropy is removed and the planar Mn AFM structure cants to produce a net Mn moment along the field direction. Below \(T_C\), the net development of in-plane Mn moment is suppressed by partially frustrated exchange interactions at the AFM-SMR/FM-SRO interfaces and competing Mn-Ru anisotropies. Hysteretic magnetization curves show a two-step magnetization reversal and enhanced coercivity. X-ray measurements confirm that the low-field magnetization reversal coincides with "free" Ru moments inside the SRO layers and that the high-field magnetization reversal involves the interfacial magnetization in the SMO layers and provide strong evidence for the presence of pinned SRO moments at the SRO/SMO interface.

\(^1\)Work supported by the Institute for NanoScience, Engineering and Technology - U.S. Department of Education and the U.S. Department of Energy, Office of Science, under Contract No. DE-AC02-06CH11357.

2:03PM Q30.00011 Electrically controlled magnetization in tricolar superlattices\(^1\), JAEKWANG LEE, NA SAI, ALEXANDER A. DEMKOV, The University of Texas — With recent breakthroughs in fabricating high-quality oxide films, ultra thin ferroelectric (FE) films have attracted significant attention. Many FE-based electronic devices proposed to date have a capacitor configuration, where a FE layer is inserted between two identical metal electrodes. We consider theoretically so-called tricolor structures or asymmetric capacitors with one electrode being ferromagnetic and other normal metal. An interesting aspect of a tricolor structure is breaking of the inversion symmetry which is expected to generate new properties. The perfect conducting state may be extremely fragile to finite temperature, finite driving electric fields, finite driving frequencies, or disorder, so it will often be difficult to see experimentally. We will discuss possible experimental realizations of the phenomena

\(^1\)Supported by the ONR under grant N000 14-06-1-0362
Mott transition between a spin-liquid insulator and a metal in three dimensions, DANIEL PODOLSKY, ARUN PARAMEKANTI, YONG BAEK KIM, University of Toronto, T. SENTHIL, Massachusetts Institute of Technology — We study a bandwidth controlled Mott metal-insulator transition (MIT) between a Fermi liquid metal and a quantum spin-liquid insulator at half-filling in three dimensions (3D). Using a slave rotor approach, and incorporating gauge field fluctuations, we find a continuous MIT and discuss the finite temperature crossovers around this critical point. We show that the specific heat $C \sim T \ln T$ at the MIT and argue that the electrical transport on the metallic side near the transition should exhibit a 'conductivity minimum' as a function of temperature. A possible candidate to test these predictions is the 3D spin liquid insulator Na$_4$Ir$_5$O$_9$ which exhibits a pressure-tuned transition into a metallic phase. We also present the electron spectral function of Na$_4$Ir$_5$O$_9$ at the transition.

Lattice vibration modes in CdCr$_2$O$_4$, J.-H. KIM, S.-H. LEE, University of Virginia, M. MATSUDA, JAEA, Japan, H. UEDA, Y. UEDA, ISSP, University of Tokyo, J.-H. CHUNG, Korea University, Korea, S. TSUTSUI, A. BARON, SPring8, Japan — In geometry frustrated magnets, spin-lattice coupling can play an important role in lifting the magnetic frustration. In order to understand the mechanism, we have performed inelastic synchrotron x-ray measurements on a single crystal of a frustrated magnet CdCr$_2$O$_4$ that undergoes such a three-dimensional spin-Peierls phase transition at $T_N = 12.5$ K. Our data taken above and below $T_N$ could be well explained by the rigid ion model, which led to a full identification of the lattice vibration modes in CdCr$_2$O$_4$. A phonon anomaly that might be associated with the transition, however, was not observed.

Crystal and magnetic structures of the three-dimensional spin-Peierls phase transition at $T_N = 12.5$ K from a cubic paramagnetic state to a tetragonal Neel state. The exact nature of the lattice distortion, and the one-to-one correspondence between the distortion and the magnetic ground state has been a long-standing issue. To unveil the mystery, we have performed synchrotron x-ray diffraction measurements on a single crystal of this compound and neutron diffraction measurements on a powder sample. Our detailed analysis of the single crystal x-ray data shows that below $T_N$ the symmetry of the crystal structure is lowered from the cubic $Fd3m$ to the tetragonal $I4/m2$ due to formation of a complex pattern of Cr-Cr clustering. The relation between the distorted crystal structure and the magnetic structure will also be discussed.

Magnetic Correlations in YBaCo$_4$O$_7$: A Frustrated Magnet with Novel Trigonal Bipyramidal Chains, JOHN MITCHELL, Argonne National Laboratory, PASCAL MANUEL, LAURENT CHAPON, ISIS Facility, PAOLO RADAELLI, Dept. of Physics, University of Oxford, HONG ZHENG, Argonne National Laboratory — Novel structural motifs generate opportunities to explore unique geometrically frustrated groundstates and their properties. One such new material, YBaCo$_4$O$_7$ (Y114), is closely related to the pyrochlore lattice, differing only in the stacking sequence of triangular layers. This alternative stacking sequence leads to chains of corner sharing trigonal bipyramids with magnetic ion vertices, a novel motif among geometrically frustrated lattices. We have studied Y114 using single crystal neutron diffraction above its ordering temperature. Strong magnetic diffuse scattering can be understood using Monte-Carlo simulations, and a simple nearest-neighbor model explains the magnetic structure. Along the c-axis, long-range order arising from the corner-sharing bipyramids create a quasi one-dimensional order at finite temperature. In contrast, the spin-spin correlation function decays rapidly in the ab-plane, following a unique short-range configuration that enforces an Ising-like order along the b-axis. Approaches to suppressing long-range order in the system will be discussed.

Specific heat of gadolinium garnets, JEFFREY QUILLIAM, SHUCHAO MENG, Department of Physics and Astronomy and Institute for Quantum Computing, University of Waterloo, Waterloo, ON, Canada, LINTON CORRUCCINI, Physics Department, University of California-Davis, Davis, California, USA, OLEG PETRENKO, Department of Physics, University of Warwick, Coventry, United Kingdom, MICHEL GINGRAS, Department of Physics and Astronomy, University of Waterloo, Waterloo, ON, Canada; Canadian Institute for Advanced Research, Toronto, ON, Canada, JAN KYCIA, Department of Physics and Astronomy and Institute for Quantum Computing, University of Waterloo, Waterloo, ON, Canada — Specific heat measurements on two different geometrically-frustrated, Heisenberg, garnet lattices will be presented. The specific heat of a compound of gadolinium garnets, GGG, is found to be consistent with previous measurements of the specific heat of GGG and shows no signs of a standard ordering anomaly despite sharp Bragg peaks that were seen in neutron diffraction experiments. A first measurement of the specific heat of polycrystalline Gd$_3$Li$_2$Te$_3$O$_{12}$, in contrast, shows a sharp first-order phase transition at 240 mK. We will discuss possible explanations for such diverse behavior in very similar systems.
12:39 PM Q31.00008 Long-range antiferromagnetic interactions in ZnFe$_2$O$_4$ and CdFe$_2$O$_4$ . CHING CHENG, Department of Physics, National Cheng Kung University, Taiwan, Taiwan. CHING-SHENG LIU, Yu-Jia Junior High School, Luzhu Shiang, Kaohsiung County 82143, Taiwan, HSUEH FANG YEH, Department of Physics, National Cheng Kung University, Tainan, Taiwan. For the first time, the Fe-Fe interactions in the well known geometrically frustrated antiferromagnets of Zn and Cadmium ferrite are determined quantitatively by considering structures of different collinear magnetic distributions using first-principles methods. Both the generalized gradient approximation (GGA) and GGA plus the onsite Coulomb interaction (GGA+U) are considered for the exchange-correlation energy functional. The interactions up to third neighbors are determined to be all antiferromagnetic regardless of which approximation scheme (GGA or GGA+U) is used. Surprisingly, the third neighbor interaction is much stronger than the second-neighbor one. The magnetic distributions have prominent effects on energies as well as density of states, including band gaps, for both normal and inverse spinel structures of these two materials. The possible magnetic distributions coincident with neutron scattering results are also investigated.

12:51 PM Q31.00009 Frustrated Quantum Antiferromagnetism on the Diamond Sublattice of A-site Magnetic Spinels . LEON BALENTS, Kavli Institute for Theoretical Physics, UCSB — Spinel crystals, with the chemical formula AB$_2$X$_4$, in which only the A atom is magnetic, realize antiferromagnetism on a diamond sublattice. We first discuss examples, such as CoAl$_2$O$_4$ and MnSc$_2$S$_4$, which exhibit "bond frustration" due to the competing effects of first and second neighbor interactions. This is well modeled by a classical Heisenberg Hamiltonian, which leads to a remarkable ground state degeneracy of coplanar spins, in which the wavevector of the spiral can lie anywhere on a "spiral surface" in momentum space. We describe how thermal fluctuations lead to a broad spin liquid regime, with unique properties, and magnetic ordering at low temperatures. We next discuss the intriguing case of FeSC$_2$S$_4$, in which orbital degeneracy leads to a persistent "spin orbital liquid" down to the lowest temperatures. We argue that this material is in the vicinity of an unusual quantum critical point driven by a competition between exchange and spin-orbit interactions.

1:27 PM Q31.00010 Phase competition and large residual entropy in the pyrochlore double-exchange system . YUKITOSHI MOTOME, University of Tokyo, NOBUO FURUKAWA, Aoyama Gakuin University, ERATO-MF — Strong interplay between spin and charge degrees of freedom gives rise to fascinating phenomena, in particular when the system undergoes severe geometrical frustration, such as anomalous magneto-transport and heavy-mass behavior. We investigate this intriguing problem in the double-exchange model on the frustrated pyrochlore lattice by employing an unbiased Monte Carlo simulation. We find that as increasing the antiferromagnetic superexchange between localized moments, the ferromagnetic metallic state stabilized by the double-exchange mechanism becomes unstable, and is taken over by a paramagnetic metal in which spin correlations are strongly suppressed by the frustration. The critical field displays a novel and generic behavior, which can be tuned by chemical doping. We describe inelastic neutron scattering measurements on powder samples of IPA-Cu$_2$Br$_{12}$-tetrakis thiourea (DTN). In absence of doping, this compound clearly displays field-induced Bose-Einstein condensation of magnons [V. Zapf et al., Phys. Rev. Lett. 98, 047205 (2007)], as revealed by the mean-field scaling of the field-induced ordering temperature, $T_c \sim \left| H - H_c \right|^\phi$ with $\phi = 2/3$. The critical field $H_c$ corresponds to a $T = 0$ quantum phase transition (QPT) between a spin gap phase and a gapless ordered phase. Here we show that site dilution opens a novel gapless spin-liquid phase close to the ordering transition, corresponding to a Bose glass phase of localized magnons. Disorder leads to a radical change in the universality class of the QPT (which turns into a quantum percolation transition), and in the critical temperature scaling, which exhibits a novel universal exponent $\phi = 1.2$. A crossover to mean-field scaling of $T_c$ at finite temperature is observed, and explained via a scenario of thermal percolation of magnons.

1:39 PM Q31.00011 Magnetic Bose condensation vs. magnon localization in a model magnet with site dilution . TOMMASO ROSCILDE, Ecole Normale Superieure - Lyon, STEPHAN HAAS, University of Southern California, RONG YU, University of Tennessee - Knoxville — We report on the theoretical field-temperature phase diagram of anisotropic coupled S=1 chains with site dilution, modeling the magnetic behavior of doped NiAl$_2$-tetrakis thiourea (DTN). In absence of doping, this compound clearly displays field-induced Bose-Einstein condensation of magnons [V. Zapf et al., Phys. Rev. Lett. 98, 047205 (2007)], as revealed by the mean-field scaling of the field-induced ordering temperature, $T_c \sim \left| H - H_c \right|^\phi$ with $\phi = 2/3$. The critical field $H_c$ corresponds to a $T = 0$ quantum phase transition (QPT) between a spin gap phase and a gapless ordered phase. Here we show that site dilution opens a novel gapless spin-liquid phase close to the ordering transition, corresponding to a Bose glass phase of localized magnons. Disorder leads to a radical change in the universality class of the QPT (which turns into a quantum percolation transition), and in the critical temperature scaling, which exhibits a novel universal exponent $\phi = 1.2$. A crossover to mean-field scaling of $T_c$ at finite temperature is observed, and explained via a scenario of thermal percolation of magnons.


Wednesday, March 18, 2009 11:15AM - 1:51PM — Session Q32 GMAG: Magnetic Domains and Domain Walls 336

11:15 AM Q32.00001 Effect of Wall Width on Spin Torque in Ferromagnetic Domain Walls . E.A. GOLOVATSKI, M.E. FLATTÉ, OSTC and Department of Physics and Astronomy, University of Iowa — The amount of spin torque exerted on a domain wall in a ferromagnetic semiconductor depends on the amount of spin flip that occurs during the transport process. Starting with a model Hamiltonian[1], we calculate the total amount of spin torque exerted on a π wall and a 2π wall for ballistic transport across the domain wall, and calculate the dependence of the torque on the width of the domain wall. In very thin 2π walls, transport occurs with almost no spin flip. As the wall width increases, spins precess more inside the domain wall, increasing the spin torque. In a π wall, where most spins will flip during transport through a thick wall, we find that the spin torque increases monotonically with wall width. In contrast, spins in a thick 2π wall will continue to precess back towards their original configuration, and there will be much less net spin torque. Thus there is very little spin torque in both very thin and very thick 2π walls, but significant spin torque is possible in a range of intermediate widths. This non-trivial dependence on the width of the domain wall leads to an optimal wall width for achieving a maximum amount of spin torque. For a 2π wall with an exchange-induced spin splitting of 100 meV, and an effective carrier mass equal to the electron mass, we calculate this optimal width to be ~ 5nm. This work was supported by an ONR MURI. [1] G. Vignale and M.E. Flatté, PRL 89, 098302 (2002).
11:27AM Q32.00002 Transport across a pinned domain wall across a GaMnAs constriction: from AMR to spin-dependent tunneling. SUNG UN CHOO, HYUNG KOOK CHOI, FABIO C.S. DASILVA, TERESA OSMINER, DAVID P. PAPPAS, YUN DANIEL PARK, DEPARTMENT OF PHYSICS AND ASTRONOMY, SEOUL NATIONAL UNIVERSITY, SEOUL 151-747, KOREA TEAM, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, BOULDER CO 80305, USA TEAM — We report on the different magnetotransport mechanism across a pinned domain wall in a GaMnAs nanowire dependent on constriction size. Nanometer-sized constrictions are realized in LT-MBE epitaxial GaMnAs by standard e-beam lithography and wet-etch processes, as well as a “break-junction” method to further decrease constriction size. Four-point probe DC IV measurements with varying angles to wire axis are utilized to study the transport mechanism— as well as magnetic properties. As constriction size approaches epitaxial thickness, nonlinear IV response is observed with a differing field dependence on temperature. As constrictions become smaller, we observe a tunneling AMR-like behavior. This effect is more evident after series of high current pulses are applied to decrease the constriction width. “Break-junction” method results in higher constriction resistances and increases in resulting MR values.

11:39AM Q32.00003 Mechanisms for low-field, and multiple domain wall injection into magnetic nanowires.1, SARAH REIFF, ANDREW KUNZ, Marquette University — The motion of a domain wall within a magnetic nanowire is important for the development of future recording, sensing and logic devices. The speed of a field driven domain wall is quickest when the applied magnetic field is below the so-called Walker Field which depends on the size and material properties of the wire. However, the field needed to inject a domain wall into a wire is much greater than the Walker Field. This discrepancy between the Walker Field and the injection field has not been well understood. By using MOKE with complicated domain wall structures, we present Landau-Lifshitz simulation results showing a significant decrease in the field needed to inject a domain wall into the wire for a variety of injection designs including: pads, rings, straight ends, and tapered ends. We also find that by applying a transverse field the required driving field to inject the wall decreases, and that the domain wall motion in the wire is faster. The magnetization of the pad and ring injection designs can be easily manipulated so that multiple walls with a known magnetization structure are injected allowing for faster, more reliable domain wall motion.

11:51AM Q32.00004 The influences of transverse magnetic anisotropy on field-induced domain wall propagation in magnetic nanowires, JIE LU, PENG YAN, XIANGRONG WANG, Physics Department, the Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong SAR, China, MICRO-MAGNETIC SIMULATION TEAM — Domain wall (DW) propagation in magnetic nanowires is an important subject in nanomagnetism because of its fundamental interest and potential applications in spintronic devices. It is well known that a head-to-head (or tail-to-tail) domain wall in a nanowire will propagate along the wire under an axial magnetic field. In this talk, we shall show that a new velocity-field formula can fit well with numerical results obtained from the open-source micromagnetic simulation package OOMMF. The fitting parameters have clear physical meanings that relate to the transverse magnetic anisotropy. How the transverse magnetic anisotropy, which can be modified by both transverse magnetic field and the aspect ratio of wire cross section, affects the DW structure and hence the DW propagation velocity will be discussed systematically.

12:03PM Q32.00005 Near-field interaction between domain walls in adjacent permalloy nanowires , LIAM O’BRIEN, Imperial College London, D. PETITT, H. T. ZENG, D. READ, E. R. LEWIS, R. P. COWBURN — Proposed data storage schemes based on ferromagnetic nanowires rely on the controlled propagation of domain walls (DWs) along nanoscale shift registers [Allwood et al. Science 309, 1688 (2005)]. To make technologically relevant devices, these nanowires must be fabricated to within a wire width of one another. However, the effect of magnetic anisotropy, which arises from the interaction between DWs in nanowires, has not been addressed. We have experimentally observed the interaction between two DWs of opposite charge travelling in adjacent permalloy nanowires (8nm thick, 100 nm wide), with inter-wire separation between 125 and 13nm. For the smallest separations, depinning fields (H_D) as high as 93 Oe were measured. Considering the energy landscape experienced by the two DWs under the approximation they are isolated and rigid and accounting for finite temperature we can completely reproduce the experimental dependence of H_D on the inter-wire spacing. Our results suggest that the interaction causes little perturbation to the DW shape. Pining resulting from localised stray fields is of interest for studying the fundamental properties of DWs as it occurs without modification of the DW or nanowire shape. Our results suggest propagation could be compromised by DW-DW interactions unless careful DW control is used.

12:15PM Q32.00006 Control of Domain Wall Structure and Pinning In Spin-Valve Nanowires . J. SAMPAIO, L. THEVENARD, E. LEWIS, L. O’BRIEN, H.T. ZENG, D. PETITT, D. READ, R.P. COWBURN, Imperial College London — Domain walls (DWs) in magnetic nanowires are the basis for several proposed data storage devices [D Allwood et al. Science 309, 1688 (2005), SS Parkin, US Patent 6,834,005 (2004)]. Most schemes use artificial defects (ADs) to modify the potential landscape seen by the DW, and thereby control its propagation. This potential modification depends on the DW structure. Integrating the nanowire in a Spin-Valve (SV) stack allows the electrical probing of the magnetization as well as electronic integration in future devices. However, using SV systems introduces strong stray fields from the reference layer, especially on the ADs. This can significantly impact the motion of DWs. The study of the influence of transverse magnetic anisotropy on constriction size. Nanometer-sized constrictions are realized in LT-MBE epifilm SV nanowires with dimensions for which only transverse DWs are stable (200nm width, free layer 8nm Ni_{1−x}Fe_{x}, pinned layer 2nm CoFe), which is verified with micromagnetic simulations. Moreover we show DW depinning at protrusions along the wire with fields lower than that required to nucleation (80/140 Oe). These results contribute to furthering the electrical integration of DW based data storage devices.


12:39PM Q32.00008 Domain Properties of a Single Magnetic Nanorod Investigated by Cantilever Magnetometry, SANGGAP LEE, ERIC MOORE, STEVEN A. HICKMAN, JOHN A. MAROHN, Cornell University — Single Ni nanorods having 50 to 100 nm diameter were integrated as the tip of ultra-sensitive cantilevers, having a force sensitivity of 8 nN/Hz^{1/2} at 4.2 K, designed for use in scanned-probe magnetic resonance force microscopy. We measured cantilever frequency, dissipation, and frequency fluctuations as a function of magnetic field, applied along both the easy axis and the hard axis of the nanorods while the cantilevers were self-oscillated. The nanorods exhibit bulk magnetization. Hard-axis magnetization interactions between DWs in Ni nanorods have not been well defined, or studied. Using MOKE with complicated domain wall structures. We present Landau-Lifshitz simulation results showing a significant decrease in the field needed to inject a domain wall into the wire for a variety of injection designs including: pads, rings, straight ends, and tapered ends. We also find that by applying a transverse field the required driving field to inject the wall decreases, and that the domain wall motion in the wire is faster. The magnetization of the pad and ring injection designs can be easily manipulated so that multiple walls with a known magnetization structure are injected allowing for faster, more reliable domain wall motion.
12:51PM Q32.00009 Magnetic Domain Structures in an In-plane Array of Cobalt Filaments with Periodic Structures. MU WANG, WEI HAN, XIANG XIONG, Natl. Lab. Solid State Microstructures, Nanjing University — With a unique electrochemical deposition method we fabricated in-plane arrays of straight cobalt filaments with periodic corrugations over a silicon substrate without using templates. The periodic corrugations on the filaments are induced by spontaneous oscillation in electrodeposition, and the periodicity can be tuned from a few tens of nanometers to a few hundreds of nanometers by controlling the electric current in experiments. Magnetic force microscopy indicates that each corrugated structure on the film may correspond to a local single magnetic domain. When the inter-filament separation is large, the magnetic domains are regularly aligned along the filament. The domains become random when the filaments are closely packed. We suggest that our results could be helpful in understanding the evolution of magnetic domain patterns on microscopic scale and may have potential application in spintronics.

1:03PM Q32.00010 Direct evidence of imprinted vortices in exchange-biased patterned bilayer nanomagnets. J.J. KAVICH, Institut Catala de Nanotecnologia (ICN), Barcelona, Spain, G. SALAZAR-ALVAREZ, Department of Materials Science and Engineering, Royal Institute of Technology, Sweden, J. SORU, Departament de Fisica, Universitat Autonoma de Barcelona, Spain, A. POTENZA, Diamond Light Source, Rutherford Appleton Laboratory, UK, A. MUGARZA, S. STEFANOW, Insitut Catala de Nanotecnologia (ICN), Barcelona, Spain, J. NOGUES, P. GAMBARDELLA, Instituto Catalana de Recerca i Estudis Avancats (ICREA), Barcelona, Spain — We investigate the magnetic domain structure in lithographically patterned nanomagnet arrays using element-sensitive circularly polarized XPEEM imaging. ZFC Py/IrMn (FM/AFM) bilayer nanodot (0.5 um – 4um dia.). arrays imaged across the Fe and Ni L edges clearly demonstrate spontaneous formation of vortex states. Magnetic contrast at the Mn L edge resonance indicates that the vortex state is transferred into the underlying AFM layer. The exchange-bias, measured through magneto-optical hysteresis measurements, verifies the AFM nature of the underlying IrMn, suggesting that the imprinted vortex state is confined to the interface by local interactions of the uncompensated interfacial Mn spins with the FM Py layer.

1:15PM Q32.00011 Confinement distance of the closure structure around a single hole in a 2D magnetic thin film. M. VELEZ, G. RODRIGUEZ-RODRIGUEZ, H. RUBIO, A. PEREZ-JUNQUERA, J.I. MARTIN, J.M. ALAMEDA, Dpto. Fisica, Univ. Oviedo-CINN, 33007 Oviedo, Spain, J.V. ANGUITA, IMM-CNMCSCIC, 28760 Madrid, Spain — One common feature in many magnetic nanostructures, such as nanorings or patterned thin films [1], is the existence of non magnetic holes within the magnetic material. However, up to now, the simple problem of a a single non magnetic hole in a 2D magnetic film has received little attention, even though it is qualitatively different from the blade domains that appear such as nanorings or patterned thin films [1], is the existence of non magnetic holes within the magnetic material. However, up to now, the simple problem of a single non magnetic hole in a 2D magnetic film has received little attention, even though it is qualitatively different from the blade domains that appear around holes in 3D magnetic material. In this work [2] this basic problem has been analyzed in detail by magnetic force microscopy, micromagnetic simulations and an analytical model. The closure magnetization configuration can be described by two -1/2 half vortices located at the hole edge along the easy anisotropy axis, and confined within a distance L that is determined by the minimization of magnetostatic and anisotropy energies constrained by the magnetic charge constraint within the system. [1] A. Perez-Junquera et al, J. Appl. Phys. 99 (2006) 033902 [2] G. Rodriguez-Rodriguez et al, Phys. Rev. B (2008) in press.

1:27PM Q32.00012 A shape phase diagram for a ferromagnetic liquid drop. SHUBHO BANERJEE, TRAVIS RASOR, Rhodes College, MIKE WIDOM, Carnegie Mellon University — A ferromagnetic liquid phase has been predicted by mean field theory and computer simulations but conclusive experimental evidence is lacking. Liquids such as ferrofluids, that are suspensions of ferromagnetic particles in solvents, magnetize only in the presence of an applied magnetic field and thus are paramagnets, not ferromagnets. A ferromagnetic liquid, if it existed, would spontaneously magnetize even in the absence of a magnetic field. A droplet of such a liquid would likely not be a sphere due to the magnetostatic energies involved. These energies will induce a magnetization texture in the drop analogous to domain formation in solids. We examine possible shapes for the droplet by optimizing its shape and magnetization textures with respect to its overall energy.

1:39PM Q32.00013 GGA+U calculation of the magnetic ground state of GdB4. LEONARD KLEINMAN, MUHAMMAD HUDA, University of Texas — We have studied eight collinear and non-collinear magnetic orientations of GdB4 using the GGA + U method, without and with spin-orbit coupling, for values of U - J between 0 and 6. For U - J = 6, the value which had been found to yield the correct Gd lattice constants, we obtain GdB4 lattice constants within 0.26% of experiment. We find the magnetization lies in-plane but is collinear, in disagreement with the most recent experimental determination.

Wednesday, March 18, 2009 11:15AM - 2:03PM — Session Q33 DCMP: Superconductivity: Response to Electromagnetic Fields and Proximity Effect 403

11:15AM Q33.00001 Magnetic field dependence of the infrared transmittance of superconducting NbTiN. D.B. TANNER, J. HWANG, X. XI, H. ZHANG, University of Florida, G.L. CARR, NSLS, Brookhaven National Laboratory — Superconductivity may be destroyed by raising the temperature of the superconductor above the transition temperature or by increasing an applied magnetic field above the upper critical field. We have studied the behavior of key microscopic properties, the superconducting energy gap and the superfluid density, through far-infrared magneto spectroscopy measurements on thin-film NbTiN. The measurements were performed at the National Synchrotron Light Source, Brookhaven National Laboratory. As temperature is increased, the gap and the superfluid density are reduced, both reaching zero at Tc. The behavior with field is different. Over much of the range between 0 and 10 T, the gap is almost unchanged, while the superfluid density is reduced, roughly following the area not in vortices in the film. Only near the highest field does the superconducting gap become reduced.

Supported by the DOE through grant DE-FG02-02ER45984 at Florida and contract DE-AC02-98CH10886 at BNL.
11:27AM Q33.00002 Strong correlation effects and optical conductivity in electron doped cuprates. TANMOY DAS, R.S. MARKIEWICZ, A. BANSIL, Northeastern University — We demonstrate that most features ascribed to strong correlation effects in various spectroscopies such as angle-resolved photoemission spectroscopy (ARPES) and optical spectra of the cuprates are captured by a calculation of the self-energy incorporating effects of spin and charge fluctuations[1]. The self-energy is calculated over the full doping range of electron-doped cuprates from half-filling to the overdoped system. The spectral function reveals four subbands, two widely split incoherent bands representing the remnant of the split Hubbard bands, and two additional coherent, spin- and charge-doped in-gap bands split by a spin-density wave, which collapses at the AFM quantum critical point (QCP) in the overdoped regime. The transition between the in-gap states leads to pseudogap features in the mid-infrared region of the optical spectra, where the incoherent features persist to high doping even above the QCP, producing a remnant Mott gap. Notably, our results are also in good accord with variational cluster and quantum Monte Carlo calculations. Work supported in part by the USDOE.

11:39AM Q33.00003 A broadband microwave study of the superconducting fluctuations in 2D InOx thin films, WEI LIU, Johns Hopkins University, MINSOO KIM, TAILUNG WU, SAMBANDAMURTHY GANAPATHY, SUNY-Buffalo, PETER ARMITAGE, Johns Hopkins University — We apply a broadband microwave 'Corbino' spectrometer covering the range from 10MHz to 20GHz to the study of 2D disordered superconducting InOx thin films. Explicit frequency dependency of the superfluid stiffness and conductivity are obtained down to 270mK. The AC measurements are sensitive to different time scales of the superconducting fluctuations. A number of fluctuation regimes are investigated (gaussian fluctuations, vortex proliferation) as we cool the sample into the low-temperature Kosterlitz-Thouless-Berezinskii-like phase. We discuss our results in terms of prevailing measurements are sensitive to different time scales of the superconducting fluctuations. A number of fluctuation regimes are investigated (gaussian fluctuations, vortex proliferation) as we cool the sample into the low-temperature Kosterlitz-Thouless-Berezinskii-like phase. We discuss our results in terms of prevailing fluctuations regimes.

11:51AM Q33.00004 Time-resolved terahertz photoconductivity of insulating cuprates. AMIR FARAHANI, JESSE PETERSEN, Simon Fraser University, RUXING LIANG, University of British Columbia, J. STEVEN DODGE, Simon Fraser University — We use a visible pump, terahertz probe technique to study the photoconductivity of the undoped cuprates. We use ultrafast optical pulses (E_{pump} = 3.1 eV) to create photoexcitons in high quality single crystals of Sr2CuO2Cl2 and YBa2Cu3O6+y, and time-domain terahertz spectroscopy to probe the resulting photoconductivity. We observe a rapid onset of photoconductivity followed by a non-exponential relaxation on a picosecond timescale. This dynamics is independent of photocarrier concentration over the range of 0.2 to 1.7 percent excitations per copper atom. Assuming a quantum efficiency of unity, we infer a mobility of ~0.2 cm^2/Vs, significantly lower than the Hall mobility in chemically doped systems[1]. As the fluence is increased, there is a weak decrease in the photoconductivity amplitude. We also measured the frequency dependence of the photoconductivity in the terahertz range, and observe an increase in photoconductivity with frequency up to 600 GHz, suggesting polaronic effects.

1 Y. Ando et al. PRL 87 017001 (2001)

12:03PM Q33.00005 Magnetic field-induced modification of superfluid density and interplane spectral weight in YBa2Cu3Oy, ANDREW LAFORGE, Univ. of CA, San Diego, WILLIE PADILLA, Boston College, KENNETH BURCH, University of Toronto, ZHIQIANG LI, ALEXANDER SCHAFGANS, Univ. of CA, San Diego, KOUJI SEGAWA, YOICHI ANDO, Osaka University, Japan, DIMITRI BASOV, Univ. of CA, San Diego — We report on the interlayer infrared response of YBa2Cu3O6+y in an applied magnetic field. This study explores both the underdoped (y = 6.67 and 6.75) and optimally doped (y = 6.95) regions of the phase diagram, and includes data for fields applied both parallel to the c axis and to the CuO2 planes in this anisotropic superconductor. A sum rule analysis reveals that magnetic fields H || c eliminate the high-frequency contribution to the superfluid density, returning the system to a more BCS-like energy scale [1]. For fields H || CuO2, however, the high-energy component scales with the superfluid density, and the anomalous scheme of condensate formation is maintained, at least in underdoped y=6.67 and 6.75 samples. This behavior is discussed in relation to the change of electronic kinetic energy and the suppression of interplane phase coherence. [1] A. D. LaForge et al., Phys. Rev. Lett. 101, 097008 (2008).

12:15PM Q33.00006 A Terahertz Conductivity Study of Pseudogap Phase in Underdoped LSCO. C. C. HOMES, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, D.M. BROUN, Dept. of Physics, Simon Fraser University, Burnaby, British Columbia, RUXING LIANG, W.N. HARDY, D.A. BONN, Dept. of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia — Microwave impedance techniques have been used to determine the critical temperature (Tc), the in-plane superfluid density (ρ0), and the dc conductivity (σdc) just above Tc in a highly-underdoped sample of YBa2Cu3O6+y for y ≥ 0.333. In this state the sample may be annealed to yield different levels of chain oxygen order and electronic doping in the copper-oxygen planes, resulting in a range of Tc ≈ 2 – 17 K. The linear relation between ρ0 and Tc is observed, not in-plane superfluid density is obtained, instead ρ0 ∝ Tc^2. However, the results do follow the more general scaling relation ρ0/8 ≈ 4.4 σdc Tc extending the validity of this relation for the in-plane data by an order of magnitude. In addition, these new results now provide a region of overlap between the scaling observed in the copper-oxygen planes, and perpendicular to the planes along the poorly-conducting c axis.

1Supported by the DOE under Contract No. DE-AC02-98CH10886.
12:39PM Q33.00008 Real-time photoinduced quasi-particle relaxation of superconductors1
JIANMIN TAO, JIAN-XIN ZHU, Theoretical Division and CNLS, Los Alamos National Laboratory — Ultrafast optical phenomena are of fundamental importance in the investigation of electronic dynamics of metals and superconductors [1]. By considering a model Hamiltonian with electron-boson coupling of a superconductor exposed to a time-dependent laser field, we calculate the current density, which can be expressed in terms of the quasi-particle density matrices. The time evolution of these density matrices is derived within a mean-field approximation using the equation-of-motion approach and is numerically investigated with Runge-Kutta method. We discuss the consequence of the d-wave pairing symmetry in the quasi-particle relaxation process.


1Acknowledgment: This work was supported by DOE under Contract No. DE-AC52-06NA25396 and Grant No. LDRD-PRD X961 at LANL.

12:51PM Q33.00009 Raman scattering from the CaC6 superconductor in the presence of disorder, ALEKSEJ MIALITISIN, Rutgers University, JUN SUNG KIM, REINHARD KREMER, Max-Planck-Institut fuer Festkoerperforschung, GIRSH BLUMBERG, Rutgers University — Polarized Raman scattering has been performed on CaC6 single crystal superconductor. We identify two of the three Raman active E2u phonon modes at 440 and 1508 cm−1expected for the K3m space group of CaC6. These first order scattering modes appear along with the D and G bands around 1300 cm−1and 1600 cm−1that are similar in origin to the corresponding bands in plain graphite. The intensities of the D and G peaks in CaC6 correlate with degree of disorder. The D band arises from the double resonant Raman scattering process; its frequency shifts as a function of excitation energy with ∼35 cm−1/eV. The double resonant Raman scattering probes phonon excitations with finite wave vector q. We compare experimental results to from-first-principles calculations.

1:03PM Q33.00010 Possibility of p-wave triplet pairing in Nb/Ni bilayers, WENJIAN LU, KOOKRIN CHAR, Center for Strongly Correlated Materials Research, Department of Physics and Astronomy, Seoul National University, Seoul 151-742, Korea, Y.K. BANG, Department of Physics, Chonnam National University, Kwangju 500-757, Korea, P. SANGIOGIO, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, M.R. BEASLEY, Department of Applied Physics, Stanford University, Stanford, CA 94305 — We have experimentally investigated the density of states (DOS) in Nb/Ni (S/F) bilayers and found the anomalous double peak structure. In order to analyze the measured DOS data, we propose a theory model in which p-wave triplet pairing correlations are induced by an inhomogeneous magnetization in the ferromagnet. The induced triplet component penetrates into the ferromagnet over a long length (much larger than a characteristic length scale $L_{P} = \sqrt{D/h}$, where $D$ is the diffusion coefficient and $h$ is exchange energy). We numerically calculate the DOS of Nb/Ni bilayers based on Eilenberger equation with various parameters and discuss the unusual sub-gap structure in the DOS. We find a good qualitative and quantitative agreement between the model calculations and our measurements and therefore suggest the possibility of p-wave triplet correlations in Nb/Ni bilayers.

1:15PM Q33.00011 1D Chain of Interacting Majorana Bound States at the Edge of a Topological Insulator, VASUDHA SHIVAMOGGI, JOEL MOORE, University of California, Berkeley — We study a realization of 1d chain of Majorana bound states that consists of alternating ferromagnetic and superconducting regions at the edge of a quantum spin hall insulator. Each boundary between a ferromagnetic and superconducting region supports a Majorana bound state, and the pair-wise interaction energies have previously been calculated in the weakly interacting limit. By adjusting the phases of the order parameters in these regions, it is possible to create a Majorana bound state localized at each interface. In the limit of well separated Majorana fermion systems, the system can be mapped to the transverse field Ising model. The phases of the Majorana fermion order parameters must be drawn from essentially the same random distribution. We examine factors in an experimental system that will move the system away from the critical point, such as Coulomb interactions and breaking of the duality between the ferromagnetic and superconducting regions.

1:27PM Q33.00012 ABSTRACT WITHDRAWN

1:39PM Q33.00013 Superconducting Proximity Effect in Thin Semiconducting Films, MICHAEL VISSERS, KEVIN INDERHEES, TIM MCDARLE, STEPHANIE LAW, PAUL GOLDBART, LAURA GREENE, JIM ECKSTEIN, University of Illinois at Urbana Champaign — We report results using a novel 3 terminal device to study the influence of the superconducting proximity effect on the sheet resistance of the N-layer, Rs, as well as the junction conductance across the N-S boundary, Gc. When the N-layer is a degenerate semiconductor the changes in these quantities correlate with degree of disorder. The D band arises from the double resonant Raman scattering process; its frequency shifts as a function of excitation energy with ∼35 cm−1/eV. These first order scattering modes appear along with the D and G bands around 1300 cm−1 and 1600 cm−1 that are similar in origin to the corresponding bands in plain graphite. The intensities of the D and G peaks in CaC6 correlate with degree of disorder. The D band arises from the double resonant Raman scattering process; its frequency shifts as a function of excitation energy with ∼35 cm−1/eV. The double resonant Raman scattering probes phonon excitations with finite wave vector q. We compare experimental results to from-first-principles calculations.

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1This work was supported by NSF No. DMR-0606529.
11:15AM Q34.00001 Influence of Magnetic Domain Structure on Abrikosov Vortex Dynamics in Superconductor-Ferromagnet Hybrids1. GORAN KARAPETROV, Argonne National Laboratory — We will review the experimental and theoretical aspects of transport properties and vortex static and dynamic behaviors in normally conducting superconductor-ferromagnet hybrid structures. Magnetotransport characteristics and scanning tunneling microscopy (STM) images of vortex structures reveal rich superconducting phase diagrams in these systems. Focusing on particular combination of a Permalloy ferromagnet with a well ordered rotatable periodic stripe-like magnetic domain structure with alternating out-of-plane component of magnetization, and a small coherence length superconductor, we will find directed nucleation of superconductivity above domain wall boundaries. We will also present the use of the Center for Nanoscale Materials and the Electron Microscopy Center at UChicago Argonne, LLC, Operator of Argonne National Laboratory. Argonne, U.S. DOE Office of Science lab, is operated under Contract No. DE-AC02-06CH11357.

11:51AM Q34.00002 The influence of magnetic domain landscape on the flux pinning in ferromagnetic/superconducting bilayers. MARTA Z. CIEPLAK, Z. ADAMUS, Institute of Physics, PAS, Warsaw, Poland, M. KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France, L. Y. ZHU, C. L. CHIEN, Johns Hopkins Univ. — A line of miniature Hall sensors has been used to study the influence of the disorder in the magnetic domain landscape on flux pinning in the ferromagnetic/superconducting (F/S) bilayers. The bilayers consist of Nb as the S layer and Co/Pt multilayer with perpendicular magnetic anisotropy as the F layer, separated by a Si buffer layer to avoid the proximity effect. By changing the Pt layer thickness, the magnetic domain landscape with different degree of disorder, ranging from uniformly distributed narrow domains (quasi-ordered landscape) to highly disordered landscape with domains of different sizes, can be predefined in the F layer. The flux behavior is then measured in the superconductor creating a series of (anti)pinning channels for externally added magnetic flux quanta forcing confinement of the Abrikosov vortices and formation of quasi-1D vortex arrays. We will also discuss potential for electronic applications of ferromagnet-superconductor hybrid systems.

12:03PM Q34.00003 Soft magnetic lithography and giant magnetoresistance in superconducting/ferromagnetic hybrids. V. VLASKO-VLASOV, U. WELP, A. IMRE, D. ROSENBERG, J. PEARSON, W. KWOK, Argonne National Laboratory — We report on direct visualization confirmed by the transport measurements of strong interactions between superconducting vortices and ferromagnetic domains in bilayers of type-II SC lead films and FM Penning films with perpendicular magnetic anisotropy. Domains in permalloy formed a submicron stripe lattice that could be easily aligned in the film plane. We show that domain walls yield a robust magnetic pinning potential providing preferential vortex motion along the stripe domains. The effect is observed in a wide temperature range and results in a noticeable anisotropy of critical currents. The anisotropy increases near Tc when the core pinning becomes inefficient and the anisotropy direction is changed by reorienting the stripe domains. Such a tunable magnetic lithography is a convenient way of varying transport properties of superconductors and developing new cryotronic devices such as microscale superconducting switches and modulators. In our samples we found an unusually high magnetoresistance of 106% in the fields of <10 Oe for the currents perpendicular to the domain walls. It can be referred to the granular structure of the lead films assisting the formation of easy flux flow channels along the stripe domains. — The work was supported by the U.S. DOE Office of Science under Contract No. DEAC02-06CH11357.

12:15PM Q34.00004 Experimental approach to search magnetic pinning in YBCO films grown by chemical deposition method. CARLOS MONTON, ANNA PALAU, JONE ZABALETA, NARCIS MESTRES, TERESA PUIG, XAVIER OBRADORs, Institut de Ciencia de Materiales de Barcelona, CSIC, 08193 Bellaterra, Spain — In the last 10 years we have developed experience in generating magnetic stripe domains (F) bilayer, the superconducting properties of the S layer are sensitive to the domain pattern in the adjacent F layer.1-2 We report studies of the magnetic stripe domains and the ferromagnetic layers of YBCO trilayers (at 77K and H=0). To improve these performances specific defects were created by chemical nanostructurated routes. Interfacial pinning was obtained by the growth of nanostructured templates generated by strain induced or assisted self-assembled processes [1]. On the other hand isotropic defect pinning contribution was increased by adding nanocomposites with second phase within the YBCO matrix. These samples were grown by modified solution precursors [2] reaching the transport c% in the fields of 10 Oe for the currents perpendicular to the domain walls. — The possible origins of this behavior will be discussed.

12:27PM Q34.00005 Interplay between ferromagnetism and superconductivity at interfaces of La0.7Ca3MnO3/YBa2Cu3O7−δ/La0.7Ca3MnO3 trilayers. FELIO PEREZ, West Virginia University, EVAL BACCA, MARIA E. GOMEZ, Universidad del Valle, Colombia, HONGTAO SHI, Sonoma State University, DAVID LEDERMAN, West Virginia University — We report studies of the transport properties of the S layer sensitive to the domain pattern in the adjacent F layer.1-2 We exploit this effect to investigate Ni films, which instead of retaining in-plane anisotropy as usual, unexpectedly acquire perpendicular anisotropy when the thickness is above a critical value. Using Ni/Nb bilayers, the transport measurements show a strong suppression of the superconducting properties when the thickness of superconducting layer is reduced below 10 unit cells. However, the magnetic response out of plane shows the presence of the superconductor until 5 unit cells. The difference between the electrical characterization and the onset of the diamagnetic transition might to be related of presence of the spontaneous vortex phase in this temperature interval.

12:39PM Q34.00006 Probing the magnetic states in a ferromagnet using a superconductor. LEIYI ZHU, TINGYONG CHEN, CHIA-LING CHIEN, Department of Physics and Astronomy, Johns Hopkins University — In a superconductor (S)/ferromagnet (F) bilayer, the superconducting properties of the S layer are sensitive to the domain pattern in the adjacent F layer.1-2 We exploit this effect to investigate Ni films, which instead of retaining in-plane anisotropy as usual, unexpectedly acquire perpendicular anisotropy when the thickness is above a critical value. Using Ni/Nb bilayers, the transport measurements show a strong suppression of the superconducting properties when the thickness of superconducting layer is reduced below 10 unit cells. However, the magnetic response out of plane shows the presence of the superconductor until 5 unit cells. The difference between the electrical characterization and the onset of the diamagnetic transition might to be related of presence of the spontaneous vortex phase in this temperature interval.

1The use of the Center for Nanoscale Materials and the Electron Microscopy Center were supported by UChicago Argonne, LLC, Operator of Argonne National Laboratory. Argonne, U.S. DOE Office of Science lab, is operated under Contract No. DE-AC02-06CH11357.
12:51 PM Q34.00007 Evidence for Induced Magnetization in Superconductor/Ferromagnet Bilayers | ITAY ASULIN, OFER YULI, Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel, GAD KOREN, Department of Physics, Technion-Israel Institute of Technology, Haifa 32000, Israel, ODED MILLO, Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel — The inverse proximity effect in superconductor/ferromagnet heterostructures has been the focus of recent theoretical studies. The different approaches share the basic conclusion that a sizable magnetic moment should penetrate into the superconductor side. The sign of this moment, its spatial behavior and the actual mechanism of this effect are still controversial. Very few experimental works have provided evidence for the existence of such a magnetic moment inside the superconductor. However, the effects of such an induced magnetization on the density of states of the superconductor was not observed so far and needs further theoretical and experimental clarification. We have performed scanning tunneling spectroscopy of (001)YBa$_2$Cu$_3$O$_7$ and SrRuO$_3$ bilayers, where the SrRuO$_3$ is an itinerant ferromagnet, and found an anomalous splitting of both the gap and zero bias conductance peaks that may provide evidence for the existence of such an induced magnetic moment inside the superconductor. The relevant length and energy scales of the effect will be discussed.

1:03PM Q34.00008 Interaction between magnetism and superconductivity in La$_{0.7}$Ca$_{0.3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-x}$ multilayers | T. HU, H. XIAO, C. C. ALMASAN, Department of Physics, Kent State University, Kent, OH, 44242, USA, C. VISANI, Z. SEFRIOUI, J. SANTAMARIA, GFMC, Departamento Física Aplicada III, Universidad Complutense de Madrid, 28040 Madrid, Spain — Angular and field dependent magnetoresistance measurements were performed on La$_{0.7}$Ca$_{0.3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-x}$ (LCMO/YBCO) heterostructures below and above the superconducting transition temperature $T_s \approx 28$ K of the YBCO layer, in order to address the origin of the long range proximity effect found in these heterostructures. The proximity-induced conductance in the LCMO layer at $T < T_s$ increases significantly with decreasing temperature $T$. This magnetoresistance mechanisms show that the dissipation mechanism in the LCMO layer of thickness $L_{P}$ at $T < T_s$ is due to flux vortices that have fully spin polarizes quasiparticles in the vortex core. This clearly shows that triplet superconducting pairs penetrate into the ferromagnetic LCMO layer. An estimate of $L_{P} \approx 4.7$ nm at 10 K is in excellent agreement with a previously reported value and further shows the consistency of the present analysis.

1:15PM Q34.00009 Directional control of the inverse superconducting spin-switch | CRISTINA VISANI, NORBERT M. NEMES, MIRKO ROCCHI, CHRISTIAN MILLER, JAVIER GARCIA-BARRIOCANAL, DIEGO ARIAS, ZOUHAIR SEFRIOUI, CARLOS LEON, JACOBO SANTAMARIA, Universidad Complutense de Madrid, Spain, MAR GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid, Spain, SUSANNE G. E. TE VELTHUIS, AXEL HOFFMANN, Argonne National Laboratory, Mike R. FITZSIMMONS, Los Alamos National Laboratory — We report results on the study of spin dependent transport in La$_{0.7}$Ca$_{0.3}$MnO$_3$/YBa$_2$Cu$_3$O$_{7-x}$/La$_{0.7}$Ca$_{0.3}$MnO$_3$ multilayers, focusing on the effects induced by magnetic anisotropy of the LCMO. The study of magnetic anisotropy through the combination of transport measurements, magnetometry, x-ray magnetic circular dichroism and polarized neutron reflectometry, allowed us to unravel the origin of the inverse superconducting spin switch. Applying the magnetic field along the easy axis we obtained a plateau-like response reflecting a well defined antiparallel alignment of the LCMO layers over a wide magnetic field range yielding large magnetoresistance that we ascribe unambiguously to the spin dependent transport.

1 Work supported by Spanish MICINN and DOE-BES.

1:27PM Q34.00010 Oxide thin film based inverse superconducting spin switches | NORBERT M. NEMES, C. VISANI, C. MILLER, M. ROCCHI, F. BRUNO, J. GARCIA-BARRIOCANAL, Z. SEFRIOUI, C. LEON, J. SANTAMARIA, Universidad Complutense de Madrid, Spain, M. IGLESIAS, F. MOMPEAN, M. GARCIA-HERNANDEZ, Instituto de Ciencia de Materiales de Madrid, Spain, A. HOFFMANN, S. G. E. TE VELTHUIS, Argonne National Laboratory — Thin film F/S/F trilayers made of YBa$_2$Cu$_3$O$_7$ (S, YBCO) and La$_{0.7}$Ca$_{0.3}$MnO$_3$ (F, LCMO) behave as inverse superconducting spin switches (SSS) as the critical temperature of the superconductor depends on the relative orientation of the magnetization of the F layers in a way that the resistivity increases in the antiparallel configuration. This is caused by enhanced pair-breaking due to the spin dependent transport of quasiparticles transmitted from the ferromagnetic electrodes into the superconductor. Similar inverse SSS is obtained from exchange biased LCMO/YBCO/Cobalt trilayers with a broad AP field range. Spin diffusion across the superconductor, proximity effect at the F/S interface, stray fields due to domain walls of the ferromagnet and the magnetic anisotropy all play a role.

1 Work supported by MICINN and DOE-BES.

1:39PM Q34.00011 Direct and Inverse Spin Switch Effect in Superconducting Spin Valves | JIAN ZHU, CARL BOONE, XIAO CHENG, ILYA KRIVOROTOV, University of California, Irvine, KRIVOROTOV’S GROUP TEAM — We report the observation of direct and inverse spin switch effects in ferromagnet/ superconductor/ ferromagnet/ antiferromagnet (FM/SC/FM/AF) spin valves with FM = Ni$_{81}$Fe$_{19}$, AF = Ir$_{23}$Mn$_{77}$ and SC = Nb. In these spin valve structures, the magnetization of the free layer can be switched between parallel (P) and antiparallel (AP) orientations with respect to the orientation of the fixed layer by a small in-plane magnetic field. Near the superconducting transition temperature, the P state has a higher resistance than the AP state. This is the direct spin switch effect expected from the proximity effect in superconducting spin valves. However, if the fixed ferromagnetic layer is brought into a multi-domain state in zero magnetic field, resistance in this state becomes significantly higher than that of the P state and rapidly decreases to the P state value with increasing magnetic field. We explain this inverse spin switch effect by the formation of Néel - quasi-Néel domain wall pairs in the ferromagnetic bilayer. The Néel - quasi-Néel domain wall pairs induce stray magnetic fields with a significant component perpendicular to the plane of the sample. This field penetrates the SC and gives rise to vortex flow resistance. Our work shows that the inverse spin switch effect is magnetostatic in origin.

1:51PM Q34.00012 Even- to Odd-frequency Pair Conversion by Magnetic Interfaces in SC/N Junctions | MATTHIAS ESCHWIG, University of Karlsruhe, Germany, JACOB LINDER, Norwegian University of Science and Technology, TAKEHITO YOKOYAMA, Nagoya University, Japan, ASLE SUDBØ, Norwegian University of Science and Technology — We study the proximity-induced superconducting correlations in a ballisitic or diffusive normal metal (N) connected to a superconductor (SC) when the interface between them is spin-active. One of the hallmarks of the proximity effect in a non-magnetic bilayer is a minigap in the density of states of the normal metal. It scales with the Thouless energy of the normal metal and with the transmission probability of the interface. For a spin-active interface, the transmission properties of spin↑ and spin↓ electrons into N are different, giving rise to spin-dependent phase shifts at the interface. This leads to a rather surprising result. Remarkably, for any interface spin polarization there is a critical interface resistance, above which the conventional singlet proximity component vanishes at the chemical potential, while an odd-frequency triplet component remains finite. At the same time, the minigap is replaced by a low-energy band with enhanced density of states. We propose a way to unambiguously observe the odd-frequency component.

3 We acknowledge support by the DFG-CFN (ME), the Norwegian Research Council (JL, AS), and the JSPS (TY).
which is ascribed to the change of the Fermi-surface structure by the electron doping. As for the superconducting properties for $T_c$ and pseudogap behavior is observed in $30\, K$, suggesting the development of AFM spin fluctuations with decreasing temperature. The AFM fluctuations are significantly suppressed with F-doping, We have measured the temperature-dependence of Fe-

photoluminescence spectroscopy (XPS) techniques to investigate the core-level x-ray photoemission spectra for high-temperature superconductivitor iron arsenide

LA 70803, USA, DARWIN URBINA, Department of Physics, Florida International University, Miami, FL 33199, USA, H. DING, GENFU CHEN, N.L. WANG, (Ba$_{1-x}$K$_x$)$_2$Fe$_2$As$_2$, and Other Novel Superconductors X: Spectroscopy

11:15AM Q35.00001 NMR Studies of Iron-Oxynitride Superconductor LaFeAs(O$_{1-x}$F$_x$), KENJI

ISHIDA, Department of Physics, Graduate School of Science, Kyoto University — We present experimental results of $^{75}$As and $^{119}$La nuclear magnetic resonance (NMR) in the layered oxynitride system LaFeAs(O$_{1-x}$F$_x$) ($x = 0.0, 0.04, 0.07, 0.11$ and $0.14$) where superconductivity occurs in $x$ greater than $0.04$ [1,2]. In the undoped LaFeAsO, $1/T_1$ of $^{119}$La exhibits a distinct peak at $T_{N} \approx 142\, K$ below which the La-NMR spectra become broadened due to the internal magnetic field attributed to an antiferromagnetic (AFM) ordering[1]. In the $x=0.04$ sample, $1/T_1T$ of $^{75}$As exhibits a Curie-Weiss temperature dependence down to $30\, K$, suggesting the development of AFM spin fluctuations with decreasing temperature. The AFM fluctuations are significantly suppressed with F-doping, and pseudogap behavior is observed in $1/T_1T$ in the $x=0.11$ sample with a gap value of $\Delta_{PG} \sim 175\, K$[1]. The spin dynamics vary markedly with F-doping, which is ascribed to the change of the Fermi-surface structure by the electron doping, as well as for the superconducting properties for $x=0.04, 0.07$ and $0.11$, $1/T_1$ of $^{75}$As in all compounds does not exhibit a coherence peak just below $T_c$, and follows a $T^3$ dependence at low temperatures. These results seemingly suggest that unconventional superconductivity with zero gap along lines, whereas the lack of the residual density of states at the low temperatures is incompatible with the presence of the line-nodes. We discuss similarity and difference between LaFeAs ($O_{1-x}F_x$) and cuprates, and also discuss the relationship between spin dynamics and superconductivity on the basis of F-doping dependence of $T_c$ and $1/T_1$[2].

11:51AM Q35.00002 Electron itinerancy and Strong Itinerant Spin Fluctuations in the Normal State of CeFeAsO$_{0.89}$F$_{0.11}$ Iron-Oxynitrides, F. BONDINO, E. MAGNANO, M. MALVESTUTO, F. PARMIGIANI, M.A. MCGUIRE, A.S. SEFAT, B.C. SALES, R. JIN, D. MANDRUS, E.W. PLUMMER, D.J. SINGH, N. MANNELLA — The recent discovery of high-temperature superconductivity in iron-oxynitrides and related materials has generated enormous excitement in the community. The electronic structure of the normal state of CeFeAsO$_{0.89}$F$_{0.11}$ has been measured with photoemission spectroscopy (PES) and x-ray absorption spectroscopy (XAS). The Fe XAS and PES spectra do not display satellite features commonly found in the Cu spectra of cuprates HTSCs, indicative of the absence of strong electron correlation and localization effects in the electronic structure.

The Fe 3$\delta$ spectra show exchange multiplets due to the coupling of the final Fe 3$\delta$ core hole state with the conduction band states, indicative of the presence of fluctuating spin moments on the Fe sites. These findings indicate that the FeSC must be considered a new class of materials, quite unlike the cuprate HTSC or conventional BCS superconductors [F. Bondino et al. http://arxiv.org/abs/0807.3781 (arXiv:0807.3781)].

12:03PM Q35.00003 Core Level and Valence Band Studies of the Novel Iron Pnictide Superconductors, DANIEL GARCIA, University of California, Berkeley, CHRIS JOZWIAK, CHOOKYU HWANG, ALEXEI FEDOROV, STEPHEN HANRAHAN, STEVEN WILSON, COSTEL ROTUNDU, BYRON FREELON, ROBERT BIRGENEAU, EDITH BOURRET-COURCHESNE, ALESSANDRA LANZARA — Towards understanding the physics of the superconducting iron pnictides, critical information can be gained through exploring the electronic structure of these novel materials. We have used photoemission spectroscopy to study the LaFeAsO$_{1-x}F_x$ and the PFeAsO$_{1-x}F_x$ superconductor. The evolution of valence band density of states, hybridization energy, Fermi surface topology and many body interaction are presented as a function of doping, photo energy and temperature. We explore the significance of these results to the question of electron correlation and spin physics in these Fe-based superconductors.

12:15PM Q35.00004 Core-level study of high-temperature superconductivity iron arsenide (Ba$_{1-x}$K$_x$)$_2$Fe$_2$As$_2$, YI LI, HAIZHONG GUO, JIANDI ZHANG, Institute of Physics, France, Physical Institute, University, Paris, ML 33199, USA, H. DING, GENFU CHEN, N.L. WANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, CAS, Beijing 100080, China — We have used high-resolution x-ray photoemission spectroscopy (XPS) techniques to investigate the core-level x-ray photoemission spectra for high-temperature superconductor iron arsenide (Ba$_{1-x}$K$_x$)$_2$Fe$_2$As$_2$ ($T_C = 32\, K$) and its parent compound BaF$_2$As$_2$. One important issue for understanding the nature of the superconductivity in the compound is the determination of the electron-electron correlation in the system which in principle should be reflected by the appearance of core-level satellites. We have measured the temperature-dependence of Fe-$1p$ and 3$\delta$ core-level spectrum in both parent and doped superconductor compounds and found that the core-level electronic structure is quite different from that observed in cuprates. The origin and nature of the core spectra in these iron-based materials will be discussed.

1This work was supported by NSF-DMR0346826 and DOD AMO-W911NF-07-0532.
12:27PM Q35.00005  $^{75}$As NMR study of spin-spin relaxation and impurity effects in (Ba,K)Fe$_2$As$_2$ and CaFe$_2$As$_2$, S. MUKHOPADHYAY, S. OH, A.M. MOUNCE, M. LEE, W.P. HALPERIN, Department of Physics and Astronomy, Northwestern University, IL, USA, A.P. REYES, P. KUHNS, National High Magnetic Field Laboratory, FL, USA, P.C. CANFIELD, N. NI, S. BUD’KO, Ames Laboratory, Iowa State University, IA, USA — We report here NMR measurements on Ba$_{0.85}$K$_{0.15}$Fe$_2$As$_2$ single crystals ($T_c \approx 30$ K) grown from Sn flux. The variations of the NMR line widths and shifts with temperature (40 – 150 K) and with applied field (6 – 14 T) are indicative of the presence of local magnetic impurities in these crystals, in contrast with crystals of CaFe$_2$As$_2$. Both the shift and line width are linearly dependent on the bulk magnetization and are sufficiently large that the impurity magnetic moments must be coupled through the hyperfine interaction to the As nuclei. However, this coupling is somewhat weaker than for impurities in YBCO and $^{17}$O NMR [1]. Measurements of the spin-spin relaxation from the Hahn echo decay envelope and CPMG sequences indicate slow magnetic fluctuations, $\approx 350$ Hz, whose origin will be discussed.


12:39PM Q35.00006 NMR study of the FeAs parent compounds, AFe$_2$As$_2$ (A=Ba,Ca), ERIC BAUER, SEUNG-HO BAEK, Los Alamos National Laboratory, NICHOLAS CURUO, U. of California, Davis, FILIP RONNING, JOE THOMPSON — We present $^{75}$As NMR results of the FeAs 122 parent compounds, AFe$_2$As$_2$ (A=Ba,Ca) single crystals. For BaFe$_2$As$_2$, we find that Sn impurities in the single crystal dramatically alter the low energy spin fluctuations and suppress the ordering temperature from 138 K to 85 K, and that the temperature dependence of the $^{75}$As NMR spectra and spin lattice relaxation rates reveal a second order phase transition to a state of incommensurate magnetic order. On the other hand, CaFe$_2$As$_2$ shows a commensurate first order magnetic transition which is coupled to the structural transition. By comparing the two compounds, we show that the static and dynamic properties of the FeAs systems is extremely sensitive to the microscopic out-of-plane structure in microscopic level. Our results may shed light on the superconductivity observed under pressure.

12:51PM Q35.00007 NMR relaxation rate in the FeAs superconductors, MEERA PARISH, Princeton University, JIANGPING HU, Purdue University, B. ANDREI BERNEVIG, Princeton University — We consider how different symmetries of the superconducting order parameter will affect the NMR spin relaxation rate in the newly discovered iron-based superconductors. We particularly focus on a nodeless order parameter of unconventional extended s-wave symmetry, which changes sign between the electron and hole Fermi surfaces. Using a two-band model, we show that the extended s-wave order parameter is consistent with the results of recent NMR measurements, which exhibit a characteristic $T_c^3$ dependence of the NMR spin relaxation rate, only if the inter-band contribution dominates the response.

1:03PM Q35.00008 Infrared properties of Sr(Fe,Ni)2As2 superconducting single crystals, KEVIN KIRSHENBAUM, Center for Nanophysics and Advanced Materials, University of Maryland at College Park, A.B. SUSHKOV, MRSEC, University of Maryland at College Park, S.R. SAHA, N.P. BUTCH, J. PAGLIONE, H.D. DREW, Center for Nanophysics and Advanced Materials, University of Maryland at College Park — We report on temperature dependence of the bulk single crystal reflectivity and transmission of thin crystals of iron pnictides Sr(Fe,Ni)$_2$As$_2$ in the broad frequency range from far infrared to UV. We will discuss our data in comparison to results of other experiments and theory.

$^1$Work supported in part by CNAM and NSF-MRSEC at UMD CP.

1:15PM Q35.00009 Nonequilibrium quasiparticle dynamics in single crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$, DARIUS TORCHINSKY, MIT, G.F. CHEN, J.L. LUO, N.L. WANG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, NUH GEDIK, MIT — We report on measurements of the quasiparticle dynamics in single-crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ in the superconducting state via ultrafast pump-probe spectroscopy. Quasiparticles are injected into the samples by ultrashort laser pulses. Once injected, they cause a reflectivity change of the sample at the laser frequency, allowing time-resolved optical measurements of their density. We describe the temperature and excitation density dependence of the quasiparticle recombination rate and discuss the implications of these measurements on the nature of the superconducting gap and the electron-phonon coupling in these materials.

1:27PM Q35.00010 Charge dynamics of the spin-density-wave state in BaFe$_2$As$_2$, F. PFUNER, L. DEGIORG1, ETH-Zurich, J.G. ANALYTIS, J.-H. CHU, I.R. FISHER, Stanford University — We report on a thorough optical investigation of BaFe$_2$As$_2$ over a broad spectral range and as a function of temperature, focusing our attention on its spin-density-wave (SDW) phase transition at $T_{SDW} = 135$ K. While BaFe$_2$As$_2$ remains metallic at all temperatures, we observe a depletion in the far infrared energy interval of the optical conductivity below $T_{SDW}$, ascribed to the formation of a pseudogap-like feature in the excitation spectrum. This is accompanied by the narrowing of the Drude term consistent with the dc transport results and suggestive of suppression of scattering channels in the SDW state. About 30% of the spectral weight in the far-infrared energy interval of the optical conductivity is affected by the SDW phase transition.

1:39PM Q35.00011 Temperature Dependent Local Structure of LaO$_{1-x}$F$_x$FeAs, T.A. TYSYN, T. WU, NJIT, J. WOCIK, B. RAVEL, NIST, A. IGNATOV, C. ZHANG, Rutgers University, Z. QIN, T. ZHOU, NJIT, S.-W. CHEONG, Rutgers University — The local structure of the parent and doped LaO$_{1-x}$F$_x$FeAs compounds were studied by x-ray absorption spectroscopy. The Fe-As correlations are well modeled by an Einstein model with no low temperature anomalies. While the Einstein temperatures are identical for the doped (11%) and undoped samples, the doped sample is found to have a lower level of static disorder in the Fe-As distribution. For the Fe-Fe correlation, doping enhances the effective Einstein temperature. Comparisons with the temperature dependent structure of the simpler FeSe$_{0.88}$ systems will be made. This work is supported by DOE Grant DE-FG02-07ER46402.

1:51PM Q35.00012 Exploring Local Density of States in FeSe-based Superconductors, D. ZHANG, C.S. TING, Texas Center for Superconductivity, University of Houston, Houston, TX 77204 — Starting from two Fe ions per unit cell and two degenerate orbitals per Fe ion, we construct an effective four-band model for the FeSe-based superconductors, which Fermi surfaces are consistent with those from the ARPES experiments and LDA calculations. The hole pockets at (0,0) and the electron pockets at ($\pi$, $\pi$) are controlled by hopping between the same orbitals on the nearest and second neighboring sites while the intervals between the inner and outer Fermi surfaces around (0,0) and ($\pi$, $\pi$) are determined by hopping between different orbitals on the same sublattice. On the basis of the mean field theory for superconductivity, we also investigate the local density of states for different pairing symmetries and compare them with the recent STM experiments.

Wednesday, March 18, 2009 11:15AM - 2:03PM –
Session Q36 DCMP: Carbon Nanotubes and Other Nanostructured Materials: Sensing, Transport, and Optical Properties 408
Oxygen attachment on the CNT surface favors an ether type bond. Two oxygen atoms attached on the CNT surface within the same carbon ring on parallel bonds are energetically the most stable attachment configuration. In an armchair CNT, oxygen attachment favors the C-C bonds orthogonal to the CNT axis. Correlated addition propagates axially along parallel orthogonal bonds. In a zigzag CNT, oxygen attachment prefers the slanted bond, and correlated addition propagates spirally along parallel slanted bonds. Closely spaced oxygen attachment on the armchair and zigzag CNT surfaces causes a dip in transmission symmetrically away from the Fermi level. A clustered group of oxygen atoms covalently attached to a single-walled metallic zigzag CNT can result in a one order of magnitude drop in transmission that is asymmetric with respect to the Fermi energy resulting in a qualitative resemblance to conductance versus gate voltage curves observed experimentally [Science 315, 77 (2007)]. Calculations use density functional theory combined with non-equilibrium Green functions.

We perform a comprehensive study of the effect of covalent oxygen attachment on the transmission of metallic carbon nanotubes (CNTs). Oxygen attachment on the CNT surface favors an ether type bond. Two oxygen atoms attached on the CNT surface within the same carbon ring on parallel bonds are energetically the most stable attachment configuration. In an armchair CNT, oxygen attachment favors the C-C bonds orthogonal to the CNT axis. Correlated addition propagates axially along parallel orthogonal bonds. In a zigzag CNT, oxygen attachment prefers the slanted bond, and correlated addition propagates spirally along parallel slanted bonds. Closely spaced oxygen attachment on the armchair and zigzag CNT surfaces causes a dip in transmission symmetrically away from the Fermi level. A clustered group of oxygen atoms covalently attached to a single-walled metallic zigzag CNT can result in a one order of magnitude drop in transmission that is asymmetric with respect to the Fermi energy resulting in a qualitative resemblance to conductance versus gate voltage curves observed experimentally [Science 315, 77 (2007)]. Calculations use density functional theory combined with non-equilibrium Green functions.
DZMITRY YAROTSKI, SVETLANA KILINA, Los Alamos National Laboratory, ALEC TALIN, Sandia National Laboratory, ALEXANDER BALATSKY, SERGEI TRETIAK, ANTOINETTE TAYLOR, Los Alamos National Laboratory — Production of carbon nanotube-based (CNT) devices holds a great promise for bringing the size of electronic circuits down to molecular scales. Recently, yet another step has been made towards achieving this goal by developing a new method for metal-semiconductor CNT separation, which relies on wrapping the CNT with ssDNA molecule[1]. Though it was shown that the outcome of the separation process strongly depends on the DNA sequence, further investigations have to be conducted to determine detailed structure of the hybrids and their electronic properties. Here, we use STM to characterize structural and electronic properties of the CNT-DNA hybrids and compare experimental results to theoretical calculations. STM images reveal 3.3 nm DNA coiling period, which agrees very well with the theoretical predictions. Additional width modulations with characteristic lengths of 1.9 and 2.6 nm are observed along the molecule itself. Although scanning tunneling microscopy confirms the presence of DNA in the hybrid and visualizes its structure, further experimental work is required to reveal the dependence of electronic properties of hybrids on their internal structure. [1] M. Zheng et al., Science 302, 1545 (2004).

12:39PM Q36.00008 Scanning Tunneling Microscopy of DNA-Carbon Nanotube Hybrids 

EDISON Z. DA SILVA, Physics Institute-USP, R. B. PONTES, Physics Institute-USP, EDISON Z. DA SILVA, Physics Institute-UNICAMP, ADALBERTO FAZZIO, ANTONIO J. R. DA SILVA, Physics Institute-USP — Performing first principles density functional theory (DFT) we calculated the electronic and transport properties of a Au thin nanowire with transition metal atoms (Mn, Fe, Ni or Co) bridging the two sides of the Au nanowire. We will show that these systems have strong spin dependent transport properties and that the local symmetry can dramatically change them, leading to a significant spin polarized conductance. This spin dependent transport is also associated with the transition metal in the nanowire, in particular with the d-level positioning. Using Co, for example[1], when the symmetry permits the mixing between the wire s-orbitals with the transition metal d-states, there are interference effects that resemble Fano-like resonances with an anisotropy of 0.07 at the Fermi level. On the other hand, if this symmetry decouples such states, we simply have a sum of independent transmission channels and the calculated anisotropy was 0.23. The anisotropies for the other transition metals, as well as calculated transmittances for two Co impurities will also be presented [1]. R. B. Pontes, E. Z. da Silva, A. Fazzio and Antonio J. R. da Silva, J. Am. Chem. Soc. 130 (30), 9897-903, 2008.

We thank FAPESP, CNPq and CAPES.

12:41PM Q36.00009 Electron Transport in Quasi-1D, DNA-Templated Nanoparticle Arrays 

M. S. FAIRBANKS, Department of Physics, University of Oregon, G. J. KEARNS, Department of Chemistry, University of Oregon, B. C. SCANNELL, Department of Physics, University of Oregon, R. T. LOFTUS, Department of Physics, University of Oregon, A. R. TAYLOR, Department of Physics, University of Oregon, J. E. HUTCHISON, Department of Chemistry, University of Oregon — Devices based on self-assembled metal nanoparticle arrays are good model systems for investigating the physics of the nanoscale regime, where size quantization effects and the Coulomb charging energy can dominate transport even at high temperatures. We apply a novel, highly parallel fabrication technique [1] that creates quasi-1D (200 nm x ~20 nm) arrays of Au nanoparticles (r = 1.8 nm) bonded to DNA between predefined electrodes. These devices are found to exhibit Coulomb blockade over a wide range of operating temperatures (0.24 K to ~80 K). We present an analysis of our results in comparison to recent theoretical predictions for 1- and 2D tunnel junction arrays and highlight some effects that arise from our devices’ particular geometry. [1] M. G. Warner, J. E. Hutchison. Nature Materials 2, 272 (2003); G. J. Kearns, et al. to be published.

1:03PM Q36.00010 Determining the optical modes of solid and core-shell nanowires using relativistic electrons. JEROME HYUN, Dept. of Physics, Cornell University, MARK LEVENDORF, Dept. of Chemistry and Chemical Biology, Cornell University, MARTIN BLOOD-FORSYTHE, Dept. of Physics, Haverford College, JIWONG PARK, Dept. of Chemistry and Chemical Biology, Cornell University, DAVID MULLER, Dept. of Applied and Engineering Physics, Cornell University — Nanowires serve as building-blocks for miniaturized optoelectronic devices. Determining the dispersion properties of the nanowires is necessary for device-engineering, but can be experimentally difficult with conventional optical techniques because of fundamental diffraction limitations. Fast electrons, on the other hand, can be focused to nanometer or sub-nanometer probes, providing spatial resolutions far superior to existing optical techniques. The time-varying Fourier components of the electron’s evanescent electric field can extend beyond the far ultra-violet regime, providing a near-field, broad-band light source. Using scanning transmission electron microscopy and electron energy loss spectroscopy, we report on the relativistic calculations and measurements of the optical eigenmodes of single Ge nanowires. We also present calculations of a dielectric core/metallic shell system, where couplings between the surface plasmonic modes and the cavity modes occur. The work demonstrates a powerful optical characterization solution for nanowire systems.

1:05PM Q36.00011 ABSTRACT WITHDRAWN —

1:07PM Q36.00012 Transport properties of transition metal impurities on gold nanowires

RENATO B. PONTES, Physics Institute-USP, EDISON Z. DA SILVA, Physics Institute-UNICAMP, ADALBERTO FAZZIO, ANTONIO J. R. DA SILVA, Physics Institute-USP — Performing first principles density functional theory (DFT) we calculated the electronic and transport properties of a Au thin nanowire with transition metal atoms (Mn, Fe, Ni or Co) bridging the two sides of the Au nanowire. We will show that these systems have strong spin dependent transport properties and that the local symmetry can dramatically change them, leading to a significant spin polarized conductance. This spin dependent transport is also associated with the transition metal in the nanowire, in particular with the d-level positioning. Using Co, for example[1], when the symmetry permits the mixing between the wire s-orbitals with the transition metal d-states, there are interference effects that resemble Fano-like resonances with an anisotropy of 0.07 at the Fermi level. On the other hand, if this symmetry decouples such states, we simply have a sum of independent transmission channels and the calculated anisotropy was 0.23. The anisotropies for the other transition metals, as well as calculated transmittances for two Co impurities will also be presented [1]. R. B. Pontes, E. Z. da Silva, A. Fazzio and Antonio J. R. da Silva, J. Am. Chem. Soc. 130 (30), 9897-903, 2008.

We thank FAPESP, CNPq and CAPES.

1:39PM Q36.00013 Quantum simulation of four-probe measurement of carbon nanotube

ASAKO TERASAWA, KEJII TOBIMATSU, TOMOFUMI TADA, SATOSHI WATANABE, KEJII TOBIMATSU, Dept. of Materials Engineering, The Univ. of Tokyo — The four-probe method is widely used to measure the intrinsic resistance of various materials without the effects of sample-probe contacts. Recently, there have been many attempts to apply this method to nanoscale objects. Also, anomalous behaviors of nanoscale four-probe measurements were reported such as the negative four-probe resistance of single-walled carbon nanotube. To investigate quantum effects on the four-probe measurements in nanoscale, we examined the four-probe resistance of (5,5)-carbon nanotube with a vacancy or without a vacancy theoretically on the basis of density functional tight-binding method and Green’s function method. We found that the calculated four-probe resistance is sensitive to the position of the vacancy relative to the probes even when the sample-probe connections are weak. Such a behavior is unlikely to be seen in the two-probe resistance, and suggests that the four-probe resistance of nanoscale systems depend on the sample-probe geometry in a complicated manner.

This work is supported by Global COE Program for Mechanical Systems Innovation, MEXT, Japan.

1:51PM Q36.00014 Coherent Acoustic Spectroscopy of Nanorod Arrays

MASASHI YAMAGUCHI, JIANXUN LIU, DEXIAN YE, Department of Physics, Rensselaer Polytechnic Institute, TOH-MING LU, Department of Physics, Rensselaer Polytechnic Institute — Coherent acoustic transport through vertically grown nanorod array on substrate and coherent acoustic vibration of nanorod arrays are experimentally studied by using femtosecond laser based acoustic spectroscopy in GHz-THz frequency range. In nanorod materials, acoustic phonon dispersion and life time are altered by systems depend on the sample-probe geometry in a complicated manner. Here, we use STM to characterize structural and electronic properties of the nanorod arrays and compare experimental results to theoretical calculations. We have observed the transport of the coherent acoustic pulses through the nanorod arrays. The center frequency of the acoustic pulse was comparable to the diameter of the nanorods. Also, we have observed the transfer of the acoustic energy to the nanorod vibration mode while the coherent acoustic pulse propagates through. Mean-Free-Path and time of flight of the coherent acoustic phonons is determined by comparing the results of the samples with different thicknesses.
extend this technique to more realistic solutes, Ornstein-Zernike integral equations from liquid state theory are used to study hydration around small excluded
instantaneous pulse. We have shown that this propagator can be used to reconstruct the dynamical hydration around prototypical charge distributions. To
\[ \chi(\omega, r, t) \] density propagator
Seitz Materials Research Lab, G.C.L. WONG, Depts of Mat. Science Eng. and Physics, and Seitz Materials Research Lab, U of Illinois, Urbana-Champaign, M.
solutes using inelastic x-ray scattering, R. CORIDAN, N. SCHMIDT, G.H. LAI, Dept of Physics, P. ABBAMONTE, Dept of Physics,
water dynamics, as compared to purely geometric constraints such as the size and shape of the pores.
clarify the role that the chemical interaction between the water molecules and the walls of the confining host plays in determining the characteristics of the
the Relaxing Cage Model (RCM) for the dynamics of supercooled water. Because of the heterogenous environment experienced by the water molecules in the
modified sample some of the sylanol groups in the pores' wall have been substituted with methanol groups resulting in a partially hydrophobic confining surface,
high resolution quasielastic neutron scattering spectrometers we have investigated the single particle dynamics of water confined in a hydrophobically modified
Drical Sieves, ANTONIO FARAONE, NIST Center for Neutron Research and University of Maryland, YANG ZHANG, Massachusetts Institute of
impinge at the Brewster's angle and are analyzed by a polarizer. The transient ellipticity shows a refractive index change of water by thermal conductance and
generate uniform hydrophilic and hydrophobic surfaces, and these mixtures modulate hydrophobicity two-dimensionally. Probe pulses with circular polarization
Pump pulses induce heating and acoustic vibration to a Pd surface. The Pd surface is modified by thiol chemistry. Thiols with –OH and -CH₃ end groups
laser with stable difference repetition rate. Every difference repetition rate, time delay is swept the whole pulse-to-pulse interval without an optical delay stage.
water near hydrophobic and hydrophilic surfaces is investigated by femtosecond pump-probe ellipsometry. Pump and probe pulses are from a dual Ti:sapphire
Water interfaces play a central role in a wide variety of disciplines including electrochemistry, (photo-) catalysis and biophysics. Knowledge of the details of water interfacial structure is thus essential both for a fundamental understanding of this ubiquitous liquid and for a basic understanding of the many systems in which aqueous interfaces play a key role. Although considerable progress has been made in understanding of bulk water, substantially less progress has been made at the interface. Here we report a series of surface specific studies of various water interfaces using surface-specific vibrational spectroscopies, both in equilibrium and on ultrafast (femtosecond) time scales. Our approach allows us to selectively investigate the one monolayer of water molecules at the different water interfaces. Water is characterized through its O-H stretch vibration. We find that interfacial hydrogen bonding depends strongly in the type of interface. Remarkably, for the water-air interface, interfacial hydrogen bonding is very similar to that occurring in bulk.
1:15PM Q37.00001 Surveying the potential landscapes controlling the accommodation of excess electrons by water networks, MARK JOHNSTON, Yale University — We present recent results of a new experimental approach where we use in-in pump-probe methods to measure the transition states and relative energies of isomers associated with the negatively charged water clusters. First, the vibrational spectra of various isomers are systematically disentangled using hole-burning Ar predissociation spectroscopy in a triple-stage time-of-flight mass spectrometer. We then monitor the spectra of fragment ions that are created by photoevaporation of Ar atoms through the various vibrational levels identified in the spectroscopic step. The major conclusion is the weak binding isomers are readily transformed into more strongly bound forms, while the reverse process is very inefficient. We describe progress on using this strategy to identify the large amplitude motions available in the finite systems using trace isotopes.
1:15AM Q37.00004 Ultrasound dynamic study of water confined in partially hydrophobic nanosized cylindrical sieves, ANTONIO FARAONE, NIST Center for Neutron Research and University of Maryland, YANG ZHANG, Massachusetts Institute of Technology, KAO-HSIANG LIU, CHUNG-YUAN MOU, National Taiwan University, SOW-HSIN CHEN, Massachusetts Institute of Technology — Using three high resolution quasielastic neutron scattering spectrometers we have investigated the single particle dynamics of water confined in a hydrophobically modified MCM-41-S sample. This latter is a silica matrix containing cylindrical sieves with diameter < 20 Å arranged in a hexagonal geometry. In the hydrophobically modified sample some of the sylanol groups in the pores' wall have been substituted with methanol groups resulting in a partially hydrophobic confining surface, which could be used as a model system. We have been able to analyze the data in the temperature range from 300 K to 210 K using a single consistent model, the Relaxing Cage Model (RCM) for the dynamics of supercooled water. Because of the heterogeneous environment experienced by the water molecules in the pores, the relaxation dynamics show a broad distribution of relaxation times. However, the Fickian diffusive behaviour is retained. The obtained results help clarify the role that the chemical interaction between the water molecules and the walls of the confining host plays in determining the characteristics of the water dynamics, as compared to purely geometric constraints such as the size and shape of the pores.
1:03PM Q37.00003 Femtosecond Sum-Frequency Generation Studies of the Structure and Dynamics of Interfacial Water, MISCHA BONN, AMOLF — Water interfaces play a central role in a wide variety of disciplines including electrochemistry, (photo-) catalysis and biophysics. Knowledge of the details of water interfacial structure is thus essential both for a fundamental understanding of this ubiquitous liquid and for a basic understanding of the many systems in which aqueous interfaces play a key role. Although considerable progress has been made in understanding of bulk water, substantially less progress has been made at the interface. Here we report a series of surface specific studies of various water interfaces using surface-specific vibrational spectroscopies, both in equilibrium and on ultrafast (femtosecond) time scales. Our approach allows us to selectively investigate the one monolayer of water molecules at the different water interfaces. Water is characterized through its O-H stretch vibration. We find that interfacial hydrogen bonding depends strongly in the type of interface. Remarkably, for the water-air interface, interfacial hydrogen bonding is very similar to that occurring in bulk.
1:15PM Q37.00005 Dynamics of Water Confined in Partially Hydrophobic Nanosized Cylindrical Sieves, ANTONIO FARAONE, NIST Center for Neutron Research and University of Maryland, YANG ZHANG, Massachusetts Institute of Technology, KAO-HSIANG LIU, CHUNG-YUAN MOU, National Taiwan University, SOW-HSIN CHEN, Massachusetts Institute of Technology — Using three high resolution quasielastic neutron scattering spectrometers we have investigated the single particle dynamics of water confined in a hydrophobically modified MCM-41-S sample. This latter is a silica matrix containing cylindrical sieves with diameter < 20 Å arranged in a hexagonal geometry. In the hydrophobically modified sample some of the sylanol groups in the pores' wall have been substituted with methanol groups resulting in a partially hydrophobic confining surface, which could be used as a model system. We have been able to analyze the data in the temperature range from 300 K to 210 K using a single consistent model, the Relaxing Cage Model (RCM) for the dynamics of supercooled water. Because of the heterogeneous environment experienced by the water molecules in the pores, the relaxation dynamics show a broad distribution of relaxation times. However, the Fickian diffusive behaviour is retained. The obtained results help clarify the role that the chemical interaction between the water molecules and the walls of the confining host plays in determining the characteristics of the water dynamics, as compared to purely geometric constraints such as the size and shape of the pores.
1:27PM Q37.00006 Reconstructing the dynamic hydration around hydrophobic molecular solutes using inelastic x-ray scattering, R. CORIDAN, N. SCHMIDT, G.H. LAI, Dept of Physics, P. ABBAMONTE, Dept of Physics, Seitz Materials Research Lab, G.C.L. WONG, Depts of Mat. Science Eng. and Physics, and Seitz Materials Research Lab, U of Illinois, Urbana-Champaign, M. MARUCCHO, N. BAKER, Dept of Biochem. and Mol. Biophys., Center for Comp. Biology, Washington U School of Medicine. — We combine inelastic x-ray scattering (IXS) data and liquid-state theory to image the dynamical hydration structure of water solvating molecular, hydrophobic solutes. Using ‘linear response imaging’, we computationally reconstruct the Å-scale spatial and fs-scale temporal evolution of density fluctuations in water using IXS. The imaginary part of density propagator \( \chi_{2}(q,\omega) \) is directly extracted from the IXS data, and the real part recovered using Kramers-Kronig relations. The resultant complex-valued \( \chi_{2}(q,\omega) \) is the Fourier transform of the density-density response function \( \chi_{1}(r,t) \) which measures the dynamical density fluctuations of water due to a point-like instantaneous pulse. We have shown that this propagator can be used to reconstruct the dynamical hydration around prototypical charge distributions. To extend this technique to more realistic solutes, Onslein-Zernike integral equations from liquid state theory are used to study hydration around small excluded volumes. We will present results for simple geometries and discuss the implications of combining exclusion and charge.

Wednesday, March 18, 2009 11:15AM - 2:15PM —
Session Q38 DCP: Focus Session: Nanomaterials for Energy Applications II
11:15AM Q38.00001 Nanostructured Multimetallic Catalysts in Fuel Cells1, CHUAN-JIAN ZHONG, Department of Chemistry, State University of New York, Binghamton, NY 13902 — There are two major driving forces for the global interests in research and development of fuel cells: the reality that fossil fuels are running out and the increasing environmental concern over pollution from using fossil fuels. Fuel cells utilizing hydrogen as fuels represent an important form of energy because hydrogen is a highly-efficient fuel and it is environmentally clean. Fuel cells such as proton exchange membrane fuel cell and direct methanol fuel cell are attractive because of their high conversion efficiency, low pollution, lightweight, and high power density. However, one of the important challenges for fuel cell commercialization is the preparation of active, robust and low-cost catalyst which is key component in fuel cells counting for ~30% of the cost in manufacturing fuel cells. The durability of the catalysts can also be compromised by sintering and dissolution, especially at high electrode potentials or under load-cycling. We have been developing nanotechnological approaches and investigating nanostructured materials to address some of the fundamental issues in terms of catalyst activity, stability and cost. This presentation discusses recent findings of our investigations of the synthesis and processing for nanostructured catalysts with controlled size, composition, and surface properties by highlighting a few examples of bimetallic/trimetallic nanoparticles and supported catalysts. The results from the characterization of the nanoparticles and catalysts using an array of techniques and computational modeling will be discussed. The synergistic properties of the nanostructured materials in fuel cell reactions, including electrocatalytic methanol oxidation reaction and oxygen reduction reaction, will also be discussed, along with current challenges and opportunities.

1Acknowledgement: NSF-NIRT

11:51AM Q38.00002 Reticular chemistry for clean energy, OMAR YAGHI, University of California, Los Angeles — Linking molecular building blocks by strong bonds to make networks (Reticular Chemistry) has yielded a number of new classes of materials such as metal-organic frameworks, zeolitic imidazolate frameworks and covalent organic frameworks. These are new classes of porous materials in which inorganic ‘struts’ are linked by organic ‘links’ to give extended structures with surface areas greater than 5000 m2/g. Their ultra-high surface area is useful in storing hydrogen and natural gas, and for capturing carbon dioxide. Recently we have shown that MOFs can be quite effective as air purification and capture of harmful gases. This presentation will highlight the milestones and future prospects of this new field

12:27PM Q38.00003 Chemical tools for creating energy-relevant nanomaterials, RAYMOND SCHAAK, Pennsylvania State University — An important pre-requisite for using nanoscale materials in energy-related applications is the ability to make them on-demand and to rigid and pre-determined standards. For example, creating nanoscale solids with controllable composition, crystal structure, size, morphology, and surface chemistry is necessary for optimizing and fine-tuning their properties, as well as spatially organizing them and interfacing them with other components in a device. This talk will summarize our efforts to controllably and rationally synthesize shape-controlled nanocrystals of complex multi-element metallic and semiconductor materials. Collectively, these results provide reliable and predictable guidelines for designing and synthesizing complex nanomaterials of solids that are typically viewed as challenging to make. The focus will be on applying these ideas to energy-relevant nanomaterials, including nanostructured superconductors with high critical fields, metal hydrides for hydrogen storage applications, nanoparticle catalysts relevant to fuel cells, and metal-based compounds for thermoelectric, battery, and photovoltaic applications.

1:03PM Q38.00004 Structural and electrochemical properties of V2O5 and AgV2O5 nanowires prepared by template assisted method. M.B. SAHANA, C. SUDAKAR, R. NAIK, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, V.M. NAIK, Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI 48128 — Vanadium pentaoxide and silver vanadium oxides are promising cathode materials for lithium ion battery as it allows easy intercalation/deintercalation of Li+ due its open layered structure. During Li+ intercalation energy is stored as chemical potential and during deintercalation the energy is released as electricity. Because of the large surface area nanostructured materials have enhanced energy storage capacity. We have prepared V2O5 and Ag2V2O5 (x = 0.1, 0.5) nanowires by template assisted method using radiation track etched hydrophilic PC membrane. The nanowires were grown on ITO coated glass substrates for optical analysis and on stainless steel substrate for XRD, SEM, Raman and electrochemical measurements. The effects of Ag doping on the electrochemical properties of V2O5 nanowires were investigated using a three electrode cell with nanowires as working electrode and Li as counter and reference electrode and lithium perchlorate in propylene carbonate as the electrolyte. The electrochemical characteristics of V2O5 and Ag2V2O5 nanowires such as lithium intercalation capacity, cyclic stability and diffusion coefficient will be presented.

1:15PM Q38.00005 Stable Room Temperature Hydrogen Storage in Titainum-Doped Silica, JASON SIMMONS, TANER YILDIRIM, NIST Center for Neutron Research, AHMAD HAMAED, DAVID ANTONELLI, Department of Chemistry and Biochemistry, University of Windsor — The optimum conditions for viable room temperature hydrogen storage require materials that possess isoteric heats of adsorption in between that of standard physisorbers and chemisorbers, typically in the ~20-30 kJ/mol regime. It has been theoretically predicted that transition metal atoms incorporated onto high surface area materials could enable significant room temperature storage; herein we demonstrate a possible experimental proof of these predictions. Titanium(III) complexes are grafted onto porous silica hosts, then activated to generate sites for dissociative adsorption of hydrogen gas. Using a combination of sorption measurements and inelastic neutron scattering, we show that the activated titanium provides strong hydrogen binding sites at room temperature and that adsorbed hydrogen is stable for long periods of time at ambient conditions. Further, the hydrogen can be desorbed under mild processing conditions. Neutron vibrational spectra agree well with theoretically predicted vibrational modes of the Ti—H complex. These results represent an important step towards reversible room temperature hydrogen storage.

1:27PM Q38.00006 Universal Behavior of Core-Shell Preferences in Transition-Metal Nanoparticles1, LIN-LIN WANG, DUANE D. JOHNSON, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign Transition-metal, core-shell nanoparticles are becoming ubiquitous from (electro-) catalysis to biomedical applications, due to control of size, performance, biocompatibility, and cost. We investigate 66 binary core-shell nanoparticle systems (groups 8 to 11 in the periodic table) using density functional theory (DFT) and systematically explore their segregation energies to determine core-shell preferences. We find that core-shell preferences are described by two simple factors: (1) cohesive energy (related to vapor pressure) and (2) atomic size (quantified by Wigner-Seitz radius). Core-shell preferences determined from DFT segregation energies agree with all available observations, and predict others, which can be used for design purposes. We then provide a universal description of core-shell preference via tight-binding band-energy differences that (i) quantitatively reproduces the DFT segregation energies and (ii) confirms the electronic origins for core-shell behavior.

1Funding is through the Department of Energy Catalysis (DEFG02-03ER15476), Energy (DEFC36-05GO15064) with Sandia Metal-Hydride Center of Excellence, and BES (DEFG02-03ER46026)
1:39PM Q38.00007 Catalytic Gold Nanoparticles on an Iron Oxide Surface: A Scanning Tunneling Microscopy/Spectroscopy Study

Kwang Taeg Rim, Daejin Eom, Li Liu, Elena Stolyarova, Joan Raitano, Siu-Wei Chan, Columbia University, Maria Flytzani-Stephanopoulos, Tufts University, George Flynn, Columbia University — We present a Scanning Tunneling Microscopy/Spectroscopy study of a model catalyst system consisting of supported gold nanoparticles on a reduced Fe3O4(111) surface in ultrahigh vacuum. Gold forms two electrically distinct types of nanoparticles on an iron oxide surface upon annealing a multilayer Au/Fe3O4(111). STS measurements show that large nanoparticles (∼8nm) are metallic while single gold adatoms are bonded to the oxygen sites on the Fe3O4(111) surface. Site-specific adsorption at oxygen surface atoms and the size sensitive nature of the electronic structure (Coulomb blockade) suggest that Au adatoms are positively charged. When this Au/Fe3O4(111) catalyst system is dosed with CO at 260K, there is evidence for CO adsorption at gold adatom sites. These observations are consistent with the proposal that nonmetallic, positively charged, “invisible” Au particles are the catalytically active species for the water-gas-shift reaction on Au/metal oxide surfaces. http://clippercontrols.com/info/dielectric/constant.html

1:51PM Q38.00008 Intercalation dynamics in rechargeable batteries1, Liam Stanton, Northwestern University, Martin Bazant — We consider the ion intercalation of rechargeable battery electrode particles during charging (or discharging). We have developed a general phase-field model which incorporates entropic, enthalpic and elastic effects within the particle as well as the nonlinear chemical reactions at the particle-electrolyte interface. It is shown through linear stability analysis and numerical simulations that particle size and elastic effects will decrease or even eliminate both the spinodal region and the miscibility gap in the phase diagram.

2:03PM Q38.00009 Nanowire-based solar cell fabricated by nanosphere lithography2, Oki Gunawan, Supratik Guha, IBM T.J. Watson Research Center — Nanowire (NW) structures have been predicted to provide performance enhancement for solar cells due to improved light absorption [1] and (for radial p–n junction geometry) improved carrier collection [2]. We report the development of NW-based solar cells fabricated using nanosphere lithography. This method provides a simple, scalable, low cost and high throughput technique to define large scale NW structures. The fabricated NW solar cells (0.25 µm diameter and 1.3 µm tall) on a p–Si (100) substrate show ~30 % higher short-circuit current and ~4 % higher open circuit voltage compared to the control cells (without any NWs) with baseline efficiency of 6.2 %. The reflectance and quantum efficiency spectra reveal some advantages and shortcomings of the NW-based solar cell. This work marks some progress in the development of a scalable nanowire-based solar cell and highlights some key issues such as conformal-junction formation, surface passivation, and contact formation. [1] L. Hu and G. Chen, Nano Lett. 7, 3249 (2007). [2] B. M. Kayes et. al., J. Appl. Phys. 97, 114302 (2005).


11:15AM Q39.00001 How some proteins tubulate membranes1, Patricia Bassereau, Institut Curie — Endocytosis, exocytosis, membrane transport between intracellular compartments, virus or toxin entry or exit out of the cell, all imply to deform membrane. Membrane deformation mechanisms of cell membranes by proteins are currently actively studied. Giant vesicles (GUV) are interesting model membrane systems because they are composed of a very limited number of components compared to cellular membranes. The deformations induced by the interaction with a specific protein or any other additional components to the system, can then be directly monitored and the deformation mechanism eventually understood. In this talk, we will focus on different tubular structures induced by proteins. We will show that the B-subunits of Shiga toxin or Cholera Toxin, binding to their lipid receptors, GB3 or GM1 respectively, incorporated in GUV membrane, induce negative membrane curvature and form tubular invaginations, in absence of any other cellular machinery. Tubular structures can also be obtained when molecular motors walking along microtubules exert a pulling force on the membrane of GUV. The helicoidal assembly of dynamin, a protein involved in vivo in membrane fission can also produce tubular structures. This assembly has been reconstituted around membrane nanotubes of controlled diameter; we will show that the initial tube diameter strongly influences dynamin polymerisation. In each case, a physical framework for understanding deformation mechanism will be presented.

1 Funding was provided by EMBO, HSFP, NoE SoftComp and Institut Curie.

11:51AM Q39.00002 Membrane Disruption Effects of antimicrobial Peptide Protegrin-1, Hao Wang, James Kindt, Department of Chemistry, Emory University, Atlanta, Georgia 30322, USA — Molecular dynamics simulations have been performed to better understand membrane disruption induced by antimicrobial peptide Protegrin-1 (PG-1). Two distinct setups were adopted for atomistic simulations for DMPC/PG-1 systems. One started from bilayered ribbons either with or without the PG-1 peptides embedded and another one started from random lipid mixtures in the presence of the PG-1 peptides. Line tensions deduced from the random mixtures were generally lower with the PG-1 peptides embedded in ribbon edge, which supports edge-active role of the peptides. The random mixtures self-assembled into various structures. Extended simulations are being carried out to investigate the relation between concentration of the PG-1 peptides and the resultant structures. Furthermore, coarse-grained models have been used to simulate larger DMPC bilayers with the PG-1 peptides embedded. The PG-1 peptides were found to self-assemble into clusters. However, pore formation was not observed within our simulation period up to 3 microseconds. (DMPC: 1,2-Dimyristoyl-sn-Glycero-3-Phosphocholine)

12:03PM Q39.00003 Activation Dependent Organization of T Cell Membranes, Martin Forstner, Department of Physics, Syracuse University, Björn Lillemoe, Mark Davis, Howard Hughes Medical Institute and Department of Microbiology and Immunology Stanford University School of Medicine, Jay Groves, Howard Hughes Medical Institute and Department of Chemistry University of California — We investigate the role of lipid anchor motifs in the micro-organization of T-cell plasma membranes. To that end we generated a combinatorial library of protein constructs by fusing different lipid-modification sites of lipid anchored proteins with one of two fluorescent proteins (EGFP and Cherry). Two of these constructs that encode either for myristoylation, palmitoylation, geranylation or glycosylphosphatidylinositol (GPI) elaboration were co-expressed and dual color fluorescence cross-correlation spectroscopy (FCCS) was used to exploit comovement as a signature of co-localization. We find that in living T cells most anchors only co-localize with themselves, while different anchors move independently from each other. This suggests that a variety of domains with different chemical compositions exist in the plasma membrane and that the lipid anchor structure plays a key role in domain-specific recruitment of proteins. Furthermore, the degree of aggregation is found to depend on the activation state of the T cells. Cholesterol depletion and actin-drug experiments indicate that both are involved in the dynamic organization of the T cell plasma membrane.
12:15PM Q39.00004 Blebs in Model Lipid Membranes — M. LARADJI, C.W. HARVEY, E.J. SPANGLER, University of Memphis, P.B. SUNIL KUMAR, IIT-Madras — It is now widely recognized that biomembranes exhibit complex lateral heterogeneities. Among these are blebs, which are localized balloon-like membrane protrusions observed during cell apoptosis, necrosis, and cytotoxicity. Despite the poorly understood mechanism of bleb formation and their physiological role, they recently received a renewed attention. In order to investigate the physical mechanism leading to bleb formation, we developed a model based on an implicit-solvent lipid membrane model with soft interactions recently proposed by us [J. Chem. Phys. 128, 035102 (2008)]. The model also incorporates an explicit fluctuating polymer meshwork simulating a cytoskeleton, which is anchored to the membrane. Using systematic large-scale simulations of membranes with varying values of the lipid density, cytoskeleton grafting-sites density and cytoskeleton tension, we found that localized blebs are formed on the membrane exoplasmic side in the presence of mismatch between tensions of the bare membrane and cytoskeleton. The blebs are pinned by the cytoskeleton anchors, reminiscent to those observed in apoptotic cells. The distance between neighboring anchors determines the neck of a bleb. The remaining membrane surrounding the blebs stiffens to accommodate the tensed cytoskeleton.

1:27PM Q39.00005 Membrane Fusion Proteins as Nanomachines — LUKAS TAMM, Department of Molecular Physiology & Biological Physics, University of Virginia — Membrane fusion is key to fertilization, virus infection, and neurotransmission. Specific proteins work like nanomachines to stitch together fluid, yet highly ordered lipid bilayers. The energy gained from large exothermic conformational changes of these proteins is utilized to fuse lipid bilayers that do not fuse spontaneously. Structural studies using x-ray crystallography and NMR spectroscopy have yielded detailed information about architecture and inner workings of these molecular machines. The question now is: how is mechanical energy gained from such protein transformations harnessed to transform membrane topology? To answer this question, we have determined that a boomerang-shaped structure of the influenza fusion peptide is critical to generate a high-energy binding intermediate in the target membrane and to return the “boomerang” to its place of release near the viral membrane for completion of the fusion cycle. In presynaptic exocytosis, receptor and acceptor SNAREs are zipper to form a helical bundle that is arrested shortly before the membrane. Ca binding to interlocked synaptotagmin releases the fusion block. Structural NMR and single molecule fluorescence data are combined to arrive at and further refine this picture.

1:03PM Q39.00006 Miscibility Critical Points in Plasma Membranae — BENJAMIN MACHTA, SARAH VEATCH, STEFANOS PAPANIKOLAOU, JAMES P. SETHNA, Cornell University — Lipid bilayers surround all cells and are home to a host of proteins and lipids that mediate interactions between the cell and its environment. Recent experimental work has shown that simple membranes composed of three lipid components show complex phase behavior at temperatures in the physiological range. For example, two liquid phases and a gel or solid phase are seen, and a second-order phase transition with Ising critical behavior can be reached at a boundary of the liquid-liquid coexistence region [1]. Surprisingly, membrane vesicles isolated from living cells can be tuned with a single parameter (temperature) to criticality [1]. This suggests that cell membranes in vivo sit near miscibility critical points, and may explain some of the paradoxes associated with putative lipid rafts proposed in other experiments. Here we report on work mapping phase diagrams for the simple membranes utilizing NMR and microscopy data. In addition, we use canonical models of phase transitions to understand the qualitative features of the membranes. Finally we explore ideas from information theory and self organized criticality to understand how and why real cells maintain a membrane near criticality. [1] Honerkamp-Smith, Veatch, and Keller, Biochim Biophys Acta. 2008 (in press)

1:15PM Q39.00007 Calcium-induced gel domains in bilayer – more elusive than thought — DENNIS DISCHER, DAVID CHRISTIAN, WOUTER ELLENBROEK, ANDREA LIU, MRSEC, University of Pennsylvania — As a highly bioactive divalent cation, calcium can in principle crossbridge anionic groups and induce domain formation and rigification, but past reports with lipid systems appear conflicted. We mix, as a robust model system, anionic and neutral polymer amphiphiles within vesicle and cylinder micelle morphologies and add calcium. Based on micro- measurements, calcium forms definitive crossbridges between the anionic amphiphiles, rigidifying the charged membranes across a fluid-gel transition and also leading to lateral phase separation without disrupting the assemblies. A systematic phase diagram shows that long-lived domains occur in a narrow region near the polyanion’s pK’s. The phase behavior appears well described by a relatively simple model in which – among electrostatic and entropic contributions – counterion entropy outcompetes attractive crossbridging to drive remixing of the highly charged polyacid at high pH. Initial observations extend from polymers to a polyanionic lipid involved in cell signaling [phosphatidylinositol (4,5)-bisphosphate], highlighting both the generality and limits of calcium effects.

1:27PM Q39.00008 Nonequilibrium instabilities of membranes with multiple-state active proteins — HSUAN-YI CHEN, Department of Physics and Institute of Biophysics, National Central University, Jhongli, Taiwan, ALEXANDER MIKHAILOV, Abteilung Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — We present a theoretical model for the dynamics of membranes containing active proteins that have several conformational states. The proteins are active because their conformational transition rates depend on the strength of external energy source that drives the system out of equilibrium. We show that there exist several types of nonequilibrium phase transitions for a membrane with proteins that have typical transition rates and in-plane diffusion constant.

1:39PM Q39.00009 Physical Foundations of PTEN/Phosphoinositide Interaction — ARNE GERICKE, ZHIPING JIANG, ROBERTA E. REDFERN, EDGAR E. KOOIJMAN, Kent State University, ALONZO H. ROSS, University of Massachusetts Medical School — Phosphoinositides act as signaling molecules by recruiting critical effectors to specific subcellular membranes to regulate cell proliferation, apoptosis and cytoskeletal reorganization, which requires a tight regulation of phosphoinositide generation and turnover as well as a high degree of compartmentalization. PTEN is a putative specific for the 3-phosphoinositide ring that is deleted or mutated in many different disease states. PTEN association with membranes requires the interaction of its C2 domain with phosphatidylinosine and the interaction of its N-terminal end with phosphatidylinositol-4,5-bisphosphate (PI(4,5)P2). We have investigated PTEN/PI(4,5)P2 interaction and found that Lys13 is crucial for the observed binding. We also found that the presence of cholesterol enhances PTEN binding to mixed PI(4,5)P2/POPC vesicles. Fluorescence microscopy experiments utilizing GUVs yielded results consistent with enhanced homotypic domain formation in the presence of these phospholipids. These experiments were accompanied by zeta potential measurements and solid state MAS 13P-NMR experiments aimed at investigating the ionization behavior of phosphoinositides.

1:51PM Q39.00010 Multiscale modeling of phospholipid bilayers: from explicit-solvent atom-resolution to solvent-free coarse-grained simulations — ZUN-JING WANG, MARKUS DESERNO, Carnegie Mellon University — To advance the efficiency of phospholipid bilayer simulations and permit the treatment of challenging phenomena on mesoscopic length- and time-scales, several solvent-free Coarse-Grained (CG) phospholipid bilayer models have been presented in the past ten years. Most of them were derived in a top-down scheme, aiming to qualitatively reproduce phase diagrams, binding and stretching rigidity, area per lipid, and the thickness of a generic bilayer in experiments. Here, we derive a bottom-up CG model of an implicit-solvent lipid bilayer by matching its structural and mechanical properties with that of a membrane in all-atom resolution. Besides preserving chemical specificity and quantitative accuracy, we expect to gain a more fundamental understanding of the relationship between the elastic, mechanical, and diffusive properties of implicit solvent bilayers and their underlying CG interaction potentials, specifically bonded and non-bonded forces, as well as the effective interactions replacing the solvent.
negative exponent. The decay exponent increases with w potentiation-to-depression ratio and multiplicative depression. Under realistic physiological parameters, the network was equilibrated with simulations for a physical time of days. For lower CHUN-CHUNG CHEN, DAVID JASNOW, University of Pittsburgh — We consider a network of integrate-and-fire neurons with random connections driven by small network of 32 neurons. For high state under the plasticity, for low activity evolves with either ultra-stable, chaotic or neutral dynamics. While experimental evidence has demonstrated that repeatable activity states can exist in cortical networks, it is still unclear what the spatio-temporal dynamics near these states are. To accurately address this question, the trajectories of similar, 1 ± ^* in the stationary ⋆, triggering the firing of a single neuron in a quiet network typically leads to a bursting event that lasts for seconds in a small network of 32 neurons. For high ⋆, the induced activities can persist in the network indefinitely. A mean-field theory combined with a master equation describing the distribution of synaptic weights predicts a power-law regime under the small jump assumption of synaptic weight changes. The exponents of predicted power law depends on the deviation of the mean synaptic weight from the w parameter and is to be determined self-consistently.

Wednesday, March 18, 2009 11:15AM - 2:15PM – Session Q40 DBP: Neural Computation 412

11:15AM Q40.00001 Deriving functional structure of neuronal networks from spike train data1

, SARAH FELDT, VAUGHN HETRICK, JOSHUA BERKE, MICHAL ZOCHOWSKI, University of Michigan — We present a novel algorithm for the detection of functional clusters in neural data. In contrast to many clustering techniques which convert functional interactions to topological distances to determine groupings, our algorithm directly utilizes the dynamics of the neurons to obtain functional groupings. No prior knowledge of the number of groups is needed, as the algorithm determines statistically significant clusters through a comparison to surrogate data sets. Additionally, we introduce a new synchronization measure and use this measure in the algorithm to observe known groupings in simulated data. We then apply our algorithm to experimental data obtained from the hippocampus of a freely moving mouse and show that it detects known changes in neural states associated with exploration and slow wave sleep. Finally, we show that the new synchronization measure can detect changes which are consistent with known neurophysiological processes involved in memory consolidation. 1This work was supported through an NSF Graduate Research Fellowship, NIH Grant EB003583, the Whitehall Foundation, and National Institute on Drug Abuse RO1 DA14318.

11:27AM Q40.00002 Bursting dynamics in vitro neural networks and their stimulation driven learning. Joon Ho Cho, June Hoan Kim, Kyoung J. Lee — Recent studies have indicated that recurring neural “bursts” may play an essential role in neural information processing and memory. One key element of this hypothesis involves the translation of temporal patterns of stimuli into spatiotemporally distributed information. One ideal system to investigate this issue is cultured network of neurons grown on multi-electrode array (MEA). Based on such in vitro systems, we have investigated the changes incurred by extrinsic stimuli in the spontaneously recurring bursting activities. We have employed, in particular, two-channel paired, delayed, tetanic stimuli to evoke different patterns of bursting activities. Our preliminary data suggests that the neural network can exhibit some learning behavior.

11:39AM Q40.00003 Burst switching between incoherence and synchrony NATHAN CROSBY, JOSEPH TRANQUILLO, Bucknell University — Studies of coupled oscillators often use diffusive connections to ensure that the coupled quantity is conserved. Signals between neurons, however, are not diffuse and may propagate unattenuated throughout a network. We compare diffusive and synaptic-like coupling of Hindmarsh-Rose (HMR) oscillators through numerical simulations. HMR parameters are tuned to either oscillate continuously or alternate bursts of oscillations and periods of quiescence. In diffusive coupling, two HMR units synchronize bursts and individual oscillations within a burst at nearly the same coupling strength. Synapse-like coupling, however, shows a new behavior, called burst switching, between incoherence and synchrony. For example, a bursting unit can entrain an oscillating unit of a different frequency during the burst but then force the oscillator into quiescence. Burst switching in various network topologies synchronizes inhomogeneous units for the duration of the burst, followed by a period of network quiescence and a return to incoherence. The summed activity resembles the progression of an epileptic seizure including the “spike and wave” at the transition from synchrony to quiescence.

11:51AM Q40.00004 ABSTRACT WITHDRAWN —

12:03PM Q40.00005 Trajectories through similarity space produced by local neocortical circuits1, JOHN BEGGS, WEI CHEN, JON HOBBS, AONAN TANG, Indiana University, Bloomington, BEGGS LAB TEAM — The dynamics found in local cortical networks strongly impact the types of computations they can perform. Major classes of cortical network models assume that spatio-temporal activity evolves with either ultra-stable, chaotic or neutral dynamics. While experimental evidence has demonstrated that repeatable activity states can exist in cortical networks, it is still unclear what the spatio-temporal dynamics near these states are. To accurately address this question, the trajectories of similar, but not identical, inputs must be quantified. We use 60 channel microelectrode arrays to measure spatio-temporal trajectories through similarity space at 4 ms resolution in organotypic cortical cultures and acute cortical slices. Here we show that while attractive, chaotic and neutral trajectories can exist in these networks, the average trajectory has a Lyapunov exponent near zero (0.01 ± 0.2, mean ± s.d.), indicating that neutral dynamics prevail. 1Supported by NSF, and MetaCyt funds to Indiana University from Eli Lilly Foundation.

12:15PM Q40.00006 Synaptic weight distribution under spike-timing dependent plasticity CHUN-CHUNG CHEN, DAVID JASNOW, University of Pittsburgh — We consider a network of integrate-and-fire neurons with random connections driven by noise triggered firings. The synaptic weights between the neurons are allowed to evolve under spike-timing dependent plasticity rules with additive potentiation and multiplicative depression. Under realistic physiological parameters, the network was equilibrated with simulations for a physical time of days. For lower potentiation-to-depression ratio w**, the synaptic weights forms a unimodal distribution which decays for large weights following a power law with a strong negative exponent. The decay exponent increases with w**, and runaway synaptic weights were observed as the exponent approaches −1. In the stationary state under the plasticity, for low w**, triggering the firing of a single neuron in a quiet network typically leads to a bursting event that lasts for seconds in a small network of 32 neurons. For high w**, the induced activities can persist in the network indefinitely. A mean-field theory combined with a master equation describing the distribution of synaptic weights predicts a power-law regime under the small jump assumption of synaptic weight changes. The exponents of predicted power law depends on the deviation of the mean synaptic weight from the w** parameter and is to be determined self-consistently.
tical neurons, AONAN TANG, JON HOBBS, Indiana University, WLADEK DABROWSKI, PAWEL HOTTOWY, ALEXANDER SHER, ALAN LITKE, Indiana University — Learning methods for spiking neural networks are not as well developed as the traditional neural networks that widely use back-propagation training. We propose and implement a Hebbian based learning method with winner-take-all competition for spiking neural networks. This approach is spike time dependent which makes it naturally well suited for a network of spiking neurons. Homeostasis with Hebbian learning is implemented which ensures stability and quicker learning. Homeostasis implies that the net sum of incoming weights associated with a neuron remains the same. Winner-take-all is also implemented for competitive learning between output neurons. We implemented this learning rule on a biologically based vision processing system that we are developing, and use layers of leaky integrate and fire neurons. The network when presented with 4 bars (or Gabor filters) of different orientation learns to recognize the bar orientations (or Gabor filters). After training, each output neuron learns to recognize a bar at specific orientation and responds by firing more vigorously to that bar and less vigorously to others. These neurons are found to have bell shaped tuning curves and are similar to the simple cells experimentally observed by Hubel and Wiesel in the striate cortex of cat and monkey.

12:39PM Q40.00008 Neural Decision Boundaries Predict Maximum Entropy Parameters, JEFF FITZGERALD, TATYANA SHARPEE, UCSD, The Salk Institute for Biological Studies — Previous studies have shown that the response properties of neural networks can be well described by a pairwise maximum entropy model (PMEM). The coupling constants in this model can be calculated from experimental data, but it is µ input. In the they would need to inputs are fully synchronous for the preferred direction and maximally dispersed in time for the null direction. Further, any inhibitory inputs lag excitatory inputs, as Priebe and Ferster have observed (2005). At any level of input strength, the selectivity is weak when only inhibitory inputs are considered. The inclusion of inhibition significantly strengthens selectivity, and this selectivity is preserved over a wide range of background noise levels and for short stimulus durations. We conclude that inhibition likely plays an essential role in the mechanism underlying direction selectivity.

12:51PM Q40.00009 Relationship between higher-order correlations in stimulus and information in the receptive fields of visual neurons1, RYAN ROWEKAMP, UCSD, TATYANA SHARPEE, Salk Institute — Neurons encode incoming signals in a series of spikes in the voltage trace across their cell membranes. This encoding is known to change in response to stimulus mean, variance, and power spectrum. Natural signals are known to have strong higher-than-second order correlations that cannot be described by a Gaussian distribution. To examine whether these higher-order statistics can also cause neurons to adapt their codes, we modeled the neural spike probability as an arbitrary nonlinear function with respect to two stimulus dimensions. The relevant stimulus dimensions were found as those that accounted for the largest mutual information between stimuli and spikes. We found that the contribution of the second dimension on the spike probability was stronger for natural, rather than Gaussian noise, stimuli and increased with the kurtosis of the stimulus distribution.

1Work has been supported by the NSF-sponsored Center for Theoretical Biological Physics (grant numbers PHY-0216576 and 0225630).

1:03PM Q40.00010 Robust Motion Processing in the Visual Cortex, AUDREY SEDERBERG, JULIA LIU, MATTHIAS KASCHUBE, Princeton University — Direction selectivity is an important model system for studying cortical processing. The role of inhibition in models of direction selectivity in the visual cortex is not well understood. We probe the selectivity of an integrate-and-fire neuron with a noisy background on top of a deterministic input current determined by a temporal-lag model for selectivity, including first only excitatory inputs and later both excitatory and inhibitory inputs. We find that the selectivity is weak when only inhibitory inputs are considered. The inclusion of inhibition significantly strengthens selectivity, and this selectivity is preserved over a wide range of background noise levels and for short stimulus durations. We conclude that inhibition likely plays an essential role in the mechanism underlying direction selectivity.

1:15PM Q40.00011 Rhythmogenic Neuronal Networks and k-Core Percolation, DAVID SCHWAB, ROBJIN BRUINSMAN, Department of Physics, UCLA, ALEX LEVINE, Department of Chemistry and Biochemistry, UCLA — The preBötzinger Complex (pBC) is a small (~10^2) network of identical excitatory neurons that collectively generate a temporally stable pattern of firing bursts interspersed by quiescent periods. The voltage output of this system is essential to the control of the mammalian breathing rhythm under certain physiological conditions. The network is also remarkable in that a small set of coupled identical neurons can generate a collective behavior that is not inherent in any one of them: individual neurons do not exhibit rhythmic bursting. We develop a simple model of interacting excitatory neurons that demonstrates this behavior as one of its dynamical regimes, and show that while some of its dynamic transitions can be understood in terms of mean field theory, others cannot. The non-mean-field behavior can be understood in terms of purely topological properties of random networks.

1:27PM Q40.00012 ABSTRACT WITHDRAWN

1:39PM Q40.00013 Determining information flow in networks containing one hundred neocortical neurons, AONAN TANG, JON HOBBS, Indiana University, WLADEK DABROWSKI, PAWEL HOTTOWY, ALEXANDER SHER, ALAN LITKE, JOHN BEGGS, Indiana University — How does information flow through networks of neurons? The type of network topology revealed could have important consequences for network efficiency and robustness to damage. Several tools, including transfer entropy, Granger causality, and directed information can be applied to this question. Yet indirect connections, connections with various delays, and feedback loops can complicate the task of uncovering the information flow structure. We have applied the above methods in simple validation studies, demonstrating that many of these issues can in principle be overcome. We will present preliminary results from neocortical networks of neurons recorded with a 512 electrode array.

1:51PM Q40.00014 Integration of neuroblasts into a two-dimensional small world neuronal network, CASEY SCHNEIDER-MIZELL, MICHAL ZOCHOWSKI, LEONARD SANDER, University of Michigan — Neurogenesis in the adult brain has been suggested to be important for learning and functional robustness to the neuronal death. New neurons integrate themselves into existing neuronal networks by moving into a target destination, extending axonal and dendritic processes, and inducing synaptogenesis to connect to active neurons. We hypothesize that increased plasticity of the network to novel stimuli can arise from activity-dependent cell and process motility rules. In complement to a similar in vitro model, we investigate a computational model of a two-dimensional small world network of integrate and fire neurons. After steady-state activity is reached in the extant network, we introduce new neurons which move, stop, and connect themselves through rules governed by position and firing rate.
2:03PM Q40.00015 Phase dependent and independent responses in auditory cortex, Didier Depireux, Barak Shechter, U of Maryland Medical School, THEEARLAB TEAM — Responses of auditory neurons are often characterized by their spectro-temporal receptive field (STRF). This linear measure has been shown to capture the overall trend of the response, but by its nature, it does not reflect any non-linear processing. We have recently shown that neurons in primary auditory cortex (AI) of the awake ferret respond with non-trivial nonlinearities (not solely the result of rectifying or saturating nonlinearities). We developed new techniques to reveal additional phase dependent (DC) and dependent (quadratic) tuning in the tuning of single neurons. One of the assumptions in the STRF model is that the mean firing rate (averaged over any single period of the stimulus) does not depend on the spectro-temporal modulations, but rather on the overall level of the stimulus. The phase-dependent tuning to the spectro-temporal envelope is analogous to complex visual neural responses, in which responses to an auditory grating stimulus do not depend on its spatial phase. We show the existence of neurons tuned in 1) a phase-independent manner, 2) a linear manner and 3) a quadratic manner to the time-frequency content of the spectral envelope of sounds.

1Supported by NSF DMR 0306766

Wednesday, March 18, 2009 11:15AM - 2:15PM – Session Q41 DCMP DMP: Strongly Correlated Electron Theory 413

11:15AM Q41.00001 Quantum dots: a new tool for studying quantum phase transitions (QPT), N. Roch, S. Florens, V. Bouchiat, W. Wernsdorfer, F. Balestro, Institut Neel, CNRS, Grenoble, France — QPT were studied in many different systems: spin chains, strongly correlated materials, high Tc superconductors, etc. but all the properties (magnetism, superconductivity ...) of these materials can be difficult to control. On the other hand, thanks to microelectronic technologies, it is now possible to obtain tailor-made quantum dots in which all the interactions can be tuned finely. It was then proposed by several theoretic papers [1] to use them as model systems for probing QPT. In this experimental work, we observed a screening/non screening QPT transition in a single-molecule transistor. We will present a full study as a function of magnetic field, bias voltage and temperature [2].


11:27AM Q41.00002 Signs of quantum Griffiths effects in the weak itinerant ferromagnet Ni-V, Almut Schroeder, Sara Ubaid-Kassis, Kent State University — Magnetization and ac-susceptibility data of Ni_{1-x}V_{x} alloys are presented in the vicinity of the critical concentration, x_c \approx 11\%, where the ferromagnetic transition temperature is expected to vanish. For x > x_c, power laws with unusual exponents are observed, which change with further dilution.

11:39AM Q41.00003 Effects of retardation on a system of polarized fermions, Ling Yang, University of California, Riverside, Filippos Klironomos, ENS, Lyon, France, Shan-Wen Tsai, University of California, Riverside — When fermion-fermion interactions are frequency dependent, retardation effects may play an important role in determining the phase diagram and critical energy scales of the system. These effects are particularly significant when there is competition between two or more instabilities of the Fermi liquid state. In order to elucidate these effects, we study a simple model of spinless fermions on a square lattice. We employ a functional renormalization-group method to obtain the flows of vertices and correlation functions of this system. The phase diagram, critical scales and sub-dominant types of order can be obtained this way for various types of interactions.

1Supported by NSF DMR 0306766

11:51AM Q41.00004 Phase diagram, correlation gap, and critical properties of the Coulomb glass, Matteo Palassini, Martin Goethe, University of Barcelona — We investigate the lattice Coulomb glass model in three dimensions via extensive Monte Carlo simulations. 1. No evidence for an equilibrium glass phase is found down to very low temperatures, contrary to mean-field predictions, although the correlation length increases rapidly near T = 0. 2. The single-particle density of states near the Coulomb gap satisfies the scaling law g(e,T) \sim T^{0.7}(J(e)/T) with λ \approx 2.2. 3. A charge-ordered phase exists at low disorder. The phase transition from the fluid to the charge ordered phase is consistent with the Random Field Ising universality class, which shows that the interaction is effectively screened at moderate temperature. Results from nonequilibrium simulations will be briefly discussed. Reference: M. Goethe and M. Palassini, arXiv:0810.1047

1Work supported by the Generalitat de Catalunya and the Ministerio de Ciencia e Innovacion (contracts FIS-2006-13321-C02-01 and AP2007-01005). The computations were performed on the Spanish Supercomputing Network (RES) node at Universidad de Cantabria.

12:03PM Q41.00005 Fingerprints of intrinsic phase separation in magnetically-doped 2DEG, Hanna Terletska, Vladimir Dobrosavljevic, Florida State University, National High Magnetic Field Laboratory — We theoretically study the properties of a recently observed [1] inhomogeneous phase preceding the metal-insulator transition in a magnetically-doped two-dimensional electron gas (2DEG). We show that, due to competition between (ferromagnetic) double-exchange and (anti-ferromagnetic) super-exchange, at very low carrier density such a system is unstable toward intrinsic phase separation (PS). Here, ferromagnetic carrier-rich (metallic) “droplets” emerge within a magnetically disordered carrier-poor (insulating) matrix. Our calculations indicate that this regime should display very unusual transport, featuring colossal magneto-resistance with exceptionally weak density dependence - in striking agreement with experiments [1] on CdMnTe quantum wells. Such exotic transport properties - we argue - should be considered as “fingerprint” for intrinsic phase separation, a behavior very different from situations where phase coexistence is driven by disorder due to extrinsic impurities or defects.


12:15PM Q41.00006 The Exponential Downfall of the Weak-Coupling SDW State in Chromium, Yejun Feng, Argonne National Lab, R. Jaramillo, T.F. Rosenbaum, Univ. of Chicago, J.C. Lang, Z. Islam, G. Srajer, Argonne National Lab, P.B. Littlewood, Univ. of Cambridge — Elemental chromium is the archetypical model system for itinerant antiferromagnetism. The incommensurate spin density wave state, originating from the nested Fermi surface, is readily observable with direct and scattering probes. Through a combination of low temperature cryogenic, diamond anvil cell, and synchrotron x-ray diffraction techniques, we measure directly the spin and charge order in the pure metal as it is driven towards its quantum critical point under pressure. We observe that both the spin and charge order are suppressed exponentially with pressure, well beyond the region where disorder cuts off such a simple evolution, and they maintain a harmonic scaling relationship over decades in scattering intensity. The observed exponential behavior of the order parameter follows a weak-coupling BCS theory for the ground state, even in the presence of strong pairing correlations that survive to surprisingly high temperatures and energies, as observed by inelastic scattering, transport, and thermal expansion measurements. This duality points to the fundamental issue of how mean-field behavior can describe so successfully important aspects of strongly coupled electron systems.
12:27PM Q41.00007 Nonanalytic spin susceptibility of interacting fermions away and near a fermionic quantum phase transition. DMITRII MASLOV, University of Florida, ANDREY CHUBUKOV, University of Wisconsin — We study nonanalytic paramagnetic response of an interacting Fermi system both away and in the vicinity of a fermionic quantum phase transition (QCP). Previous studies found that the spin susceptibility \( \chi \) scales linearly with either the temperature \( T \) or magnetic field \( H \) in the weak-coupling regime and that the interaction in the Cooper channel affects this scaling via logarithmic renormalization of prefactors of the \( T, |H| \) term. We show that Cooper renormalization becomes effective only at very low temperatures, which get even smaller near a QCP. We derive the thermodynamic potential as a function of magnetization and show that it contains, in addition to regular terms, a non-analytic \( |M|^4 \) term, which becomes \( M^4/T \) at finite \( T \). We consider the vicinity of a fermionic QCP by generalizing the Eliashberg treatment of the spin-fermion model to finite magnetic field, and show that the \( |M|^4 \) term crosses over to a non-Fermi-liquid form \( |M|^7/T \) near a QCP. The prefactor of the \( |M|^7/T \) term is negative, which indicates that the system undergoes a first-order rather than a continuous transition to ferromagnetism. We compare two scenarios of the breakdown of a continuous QCP: a first-order instability and a spiral phase and show that in a model with a long-range interaction in the spin channel first-order transition occurs before the spiral instability.

12:39PM Q41.00008 Fermionic propagators for 2D systems with singular interactions. TIGRAN SEDRAKYAN, ANDREY CHUBUKOV, Department of Physics, University of Wisconsin-Madison — We analyze the form of the fermionic propagator for 2D fermions interacting with massless overdamped bosons. Examples include a nematic and Ising fermionic quantum-critical points, and fermions at a half-filled Landau level. Fermi liquid behavior in these systems is broken at criticality by a singular self-energy, but the Fermi surface remains well defined. These are strong-coupling problems with no expansion parameter other than the number of fermionic species, \( N \). The two known limits, \( N >> 1 \) and \( N = 0 \) show qualitatively different behavior of the fermionic propagator \( G(\epsilon, \omega) \). In the first limit, \( G(\epsilon, \omega) \) has a pole at some \( \epsilon_k \), in the other it is analytic. We analyze the crossover between the two limits. We show that the pole survives for all \( N \), with residue \( Z = O(1) \), however at small \( N \) it only exists in a range \( O(N^2) \). At \( N = 0 \), the range collapses and the behavior of \( G(\epsilon, \omega) \) becomes analytic.

12:51PM Q41.00009 Non-Fermi-liquid behavior of quantum magnetooscillations near a quantum critical point. CHUNGWEI WANG, DMITRII MASLOV, Department of Physics, University of Florida — We study many-body effects in quantum magnetooscillations of a 2D strongly correlated system near fermionic and antiferromagnetic quantum critical points (QCP). The amplitude of magnetooscillations is determined by the electron self-energy \( \Sigma(\pi T, k, T) \) averaged over the Fermi surface, at the Matsubara frequency \( \omega = \pi T \) for \( \omega \gg \omega_c \), where \( \omega_c \) is the cyclotron frequency. The major contribution of the bosonic propagator to the electron self-energy comes from static spin fluctuations. In the spin-fermion model, the self-energy behaves as \( \propto T^2 \) in the antiferromagnetic system and as \( \propto T \) in \( T \) in the ferromagnetic system. This shows the non-Fermi-liquid temperature dependence of the self-energy near the QCP and the oscillation amplitude \( A \propto \exp\left[-2\pi(\pi T + \Sigma)/\omega_c \right] \) can be very different from the Lifshitz-Kosevich form. The momentum dependence of the self-energy contribution to the oscillation amplitude is also discussed.

1:03PM Q41.00010 Mechanism of multifractal spectrum termination at the Anderson-metal-insulator transition. MATTHEW FOSTER, COLUMBIA UNIVERSITY, SHINSEI RYU, UNIVERSITY OF CALIFORNIA, BERKELEY, ANDREAS LUDWIG, UNIVERSITY OF CALIFORNIA, SANTA BARBARA — We revisit the problem of wavefunction statistics at the Anderson metal-insulator transition (MIT) of non-interacting electrons in disordered interacting systems. We use a self-consistent mean-field theory that incorporates strong correlations and treats spatial fluctuations of the disorder, which find zero bias anomalies (ZBA) in transition metal oxides, we have performed calculations to determine the effect of strong correlations on the ZBA in disordered interacting systems. We use a self-consistent mean-field theory that incorporates strong correlations and treats spatial fluctuations of the disorder potential exactly. We discuss both the Anderson-Hubbard model and the extended Anderson-Hubbard model. We find that, even for a zero-range interaction, non-local self-energy corrections lead to the formation of an Altshuler-Aronov-like ZBA. In the extended Anderson-Hubbard model, Efros-Shklovskii-like physics much broader context of the delocalization transition of ordinary electrons in higher dimensions.

1:15PM Q41.00011 Effects of Strong Correlations on the Disorder-Induced Zero Bias Anomaly. WILLIAM ATKINSON, Trent University, YUN SONG, Beijing Normal University, SINAN BULUT, RACHEL WORTIS, Trent University — In conventional metals and semiconductors, density of states anomalies result from the interplay between disorder and interactions. Motivated by a number of experiments that find zero bias anomalies (ZBA) in transition metal oxides, we have performed calculations to determine the effect of strong correlations on the ZBA in disordered interacting systems. We use a self-consistent mean-field theory that incorporates strong correlations and treats spatial fluctuations of the disorder potential exactly. We discuss both the Anderson-Huband model and the extended Anderson-Hubbard model. We find that, even for a zero-range interaction, non-local self-energy corrections lead to the formation of an Altshuler-Aronov-like ZBA. In the extended Anderson-Hubbard model, Efros-Shklovskii-like physics dominates at large disorder.

1:27PM Q41.00012 Detrended Fluctuation Analysis for Dynamics in an Electron Glass. STEPHEN ARNASON, University of Massachusetts Boston — As a result of the correlations between electrons, electron glasses show enhanced fluctuations in conductance with a \( 1/f^\alpha \) frequency dependence. We are interested in looking at the time dependence of the fluctuation spectra as the system relaxes towards equilibrium after a discontinuous change in chemical potential. Our measurements are taken on FET structures where the conductance channel is fabricated from amorphous Indium Oxide with stoichiometry close to the superconductor to insulator transition. Changing the potential on the gate electrode allows us to change the chemical potential and we measure the resistance of the conductance channel as a function of time. In addition to the fluctuations there is a slow, logarithmic relaxation of the channel conductance. Because of this slow relaxation it is hard to characterize our signal as stationary, calling into question the application of Fourier transform based analysis techniques. One approach to coping with this problem is the subtraction of the slowly varying background before the calculation of the dissipation strength. At nonzero temperature \( T \), the linear conductance is proportional to \( \exp(-\sqrt{CE_n/\eta}) \). The decay of Friedel oscillation saturates for at distances larger than \( L_\eta \sim 1/\eta \) from the impurity.

1:51PM Q41.00014 Mapping the Driven Interacting Resonant Level Model to an Equilibrium Problem. EDUARDO NOVAIS, M.R. PLESSER, HAROLD U. BARANGER, Duke University — We map the driven Interacting Resonant Level Model (IRLM) to an equivalent statistical mechanical problem. Correlation functions in the nonequilibrium model are given, to all orders in perturbation theory, by thermal averages in the statistical system. This enables us to apply the traditional theoretical techniques for thermal problems, such as the renormalization group and diagrammatic expansions, to a far from equilibrium problem. Using these tools, we study the current as a function of bias, as well as of the interactions in the leads and the resonant level. As a simple example of a strongly interacting system far from equilibrium, the IRLM has played an important role in motivating and evaluating recent theoretical advances. We compare our new strategy to other recent proposals for studying far from equilibrium interacting systems.

2:03PM Q41.00015 Numerical study of relaxation dynamics in photoexcited states of one-dimensional Mott insulators\(^1\). HIROAKI MATSUEDA, National College of Technology, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, SADAMICHI MAEKAWA, Institute for Materials Physics, Tohoku University — We examine relaxation dynamics of one-dimensional Mott insulators after photoirradiation. This study is motivated by ultrafast metal-insulator switching seen in Sr2CuO3, halogen-bridged Ni compounds, and organic materials. In order to examine energy dissipation due to relaxation processes, we take account of strongly correlated electrons as well as environmental degrees of freedom by introducing the Hubbard–Holstein model. Then, we perform density matrix renormalization group calculations. We find quite large number of phonons excited just after irradiation even for very small electron-phonon coupling. We will discuss the nature of the phonon relaxation characteristic of strongly correlated systems, and how the relaxation is associated with other internal degrees of freedom of correlated electrons.

\(^1\)We acknowledge support from NAREGI project in Japan.

1:00PM - 1:00PM
Session S1 Poster Session III (1-4:00pm): Polymer Physics II; Phase Transitions; General Theory; Insulators and Dielectrics; Semiconductors; Supplementary Abstracts; Post-Deadline Abstracts
Exhibit Hall A

\section*{S1.00001 POLYMERIC AND ORGANIC MATERIALS II —}

\subsection*{S1.00002 Transmission Ellipsometry and X-Ray Studies on Shear Induced Order in iPP/CNT Nanocomposites\(^1\). YANIEL CABRERA, Tufts University, GEORGI GEORGIEV, Assumption College, LAUREN WIELGUS, BRENT STENGERT, ROBERT JUDITH, PEGGY CEBE, Tufts University — Polymer Carbon Nanotube Composites (PCNs) are the largest commercial application of carbon nanotubes (CNT) in the field of nanotechnology. Isotactic Polypropylene (iPP) is one of the best model systems to study in this field because iPP/CNT PCNs can form alpha, beta, and gamma crystallographic phases under a variety of crystallization conditions such as nonisothermal and isothermal melt crystallization, or application of shear. We prepared iPP/CNT nanocomposites from solution, by co-precipitation from a non-solvent. Films were made by compression molding, with 0.01 - 5.0 wt.% CNT. The morphological structure and the orientation of the crystals, and the impact of CNT on the crystallization kinetics, were evaluated using transmission ellipsometry, wide angle X-ray scattering, and differential scanning calorimetry. CNTs increase the nucleation rate for crystal formation. Ability of the CNTs to promote the formation of smectic phases in iPP will be discussed.

\(^1\)Research supported by the National Science Foundation, Polymers Program of the Division of Materials Research, through grant DMR-0602473.

\subsection*{S1.00003 Structure and applications of nanohybrid shish-kebabs. ERIC D. LAIRD, BING LI, CHRISTOPHER Y. LI, Drexel University — We describe some of the noteworthy aspects of “nanohybrid shish-kebabs” (NHSKs). NHSKs are nanostructures of polymer lamellar single-crystal structure in regular spacings (a few tens of nm) along carbon nanotubes. These novel composite materials are named for their resemblance to the classical shish-kebab structures observed in polymers crystallized in a shear flow. Morphology and growth mechanisms will be discussed: NHSK can be either 2- or 3-dimensional, and tuning of kebab diameters and spacing is made possible by careful control of the growth conditions. For single walled carbon nanotubes decorated with polyethylene, kebab diameters can be tuned through processing conditions to range from 40-250 nm. This method of functionalization demonstrates adhesion superior to that of most other noncovalent methods. The unique nanoarchitecture of NHSK creates opportunities for a wide variety of novel devices and improvements to existing technology. Thick films of these novel hybrid structures were fabricated by a simple vacuum filtration methods. Their application to electronics and chemical detection will be discussed.

\subsection*{S1.00004 Dielectric Relaxation of PVDF/STN Nanocomposites\(^1\). LEI YU, PEGGY CEBE — Dielectric relaxation behavior of poly(vinylidene fluoride), PVDF, with Lucentite\(^2\M STN nanoclay was investigated over the frequency range from 20 Hz to 1MHz. Lucentite\(^2\M STN synthetic nanoclay is based on hectorite structure with an organic modifier contained between the hectorite layers. Composition of the PVDF/STN nanocomposites ranged from 0%-10% STN by weight. Wide angle X-ray and Fourier transform infrared spectroscopy results are consistent with the conclusion that pure alpha phase is formed in PVDF film while STN 1% sample contained majority beta phase, and a tiny amount of alpha phase. When the STN content increased to 5% and 10% only the beta phase was observed. The \(\alpha\_a\) (glass transition) and \(\alpha\_c\) (crystalline) relaxation rates were plotted against the reciprocal of temperature, respectively. The dielectric result shows that the relaxation rate of the \(\alpha\_a\) relaxation, related to the motions of amorphous polymer chains, is increased by the addition of STN. However, the activation energy for the \(\alpha\_a\) relaxation, related to motions of the crystalline chains, remained unchanged with STN addition. A mechanism is proposed to interpret the relative position and interaction between PVDF chains and STN.

\(^1\)Research supported by the National Science Foundation, Polymers Program of the Division of Materials Research grant DMR-0602473.
S1.00005 Nanocomposites of Poly(vinylidene fluoride) with Multiwalled Carbon Nanotubes

WENWEN HUANG, Tufts University, KYLE EDENZON, LUIS FERNANDEZ, SHABNAM RAZMPOUR, Rochester Institute of Technology, JENNA WOOD-BURN, Gallaudet University, PEGGY CEBE, Tufts University — We report the preparation and characterization of nanocomposites of poly(vinylidene fluoride) (PVDF) with multiwalled carbon nanotubes (MWCNT) with a wide composition range, from 0.1 % to 5.0 % MWCNT by weight. Effect of uniaxial orientation by zone drawing is discussed and compared with unoriented compression molded films. Room temperature two-dimensional wide angle X-ray scattering and Fourier transform infrared spectroscopy were used for phase identification. Differential scanning calorimetry, dynamic mechanical analysis, and thermogravimetric analysis were used to study the thermal properties. Results indicate that: 1) incorporation of MWCNT in PVDF induces a small portion of beta phase crystal in the PVDF/MWCNT bulk films, while zone drawing causes a significant alpha to beta transition; 2) the thermal stability and mechanical properties are improved when MWCNT concentration increases; 3) The glass transition temperature does not change with MWCNT concentration, but a higher glass transition can be obtained by zone drawing.

1Research supported by the National Science Foundation, Polymers Program of the Division of Materials Research, through grant DMR 0704056.
2Correspondence author

S1.00006 Electrical/dielectric properties and conductivity mechanism of epoxy/expanded graphite composites

ATHANASIOS KANAPITSA, Technological Educational Institute of Lamia, EMMANUEL LOGAKIS, CHRISTOS PANDIS, POLYCARPOS PISSIS, National Technical University of Athens, NATASA JOVIC, VLADIMIR DJOKOVIC, Vinca Institute of Nuclear Sciences — In this work the electrical and dielectric properties, as well as the temperature dependence of the electrical conductivity of epoxy/expanded graphite (EG) composites, are studied by employing dielectric relaxation spectroscopy (DRS). For the preparation of the composites EG was sonicated in acetone for 10h and then the appropriate amount of epoxy resin added to the mixture. The sonication was prolonged for another 3 h. The mixture was dried at 60°C for a few hours and then the appropriate amount of hardener (triethylenetetramine) was added followed by mechanical stirring for 15 min. Finally, the mixture was cast in a glass mould and outgassed overnight at room temperature. Before they were removed from the mould, all samples were post-cured at 127°C for 10 min in air. Samples with EG weight fractions ranging from 0 to 8 wt.% were produced. Preliminary DRS results at room temperature indicate that electrical percolation threshold (p_c) lies between 3-5 wt.% EG. The influence of the EG fillers (for concentrations below p_c) on the dielectric relaxation mechanisms of the epoxy matrix, as well as the conductivity mechanism (for concentrations above p_c) are investigated.

S1.00007 Effect of interaction on the exfoliation and dispersion of a stack of platelets in a dynamic polymer matrix and solvent particles by a coarse-grained Monte Carlo simulation

BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — We consider a stack (layer) of four sheets in host matrix of mobile polymer chains and solvent particles and study their exfoliation and dispersion on a discrete lattice. Sheets and chains are created by tethering particles (nodes) by the bond-fluctuation mechanism. Each component interacts and executes their stochastic motion via Metropolis algorithm. Entropic constraints (excluded volume and entanglement) play a critical role in a relatively dense matrix. Therefore, the density of these constituents and their molecular weight are carefully selected to make this study feasible. Exfoliation of the sheets is examined by varying the interactions among different components, i.e., solvent particles, polymer chains, and platelets. The relaxation time for dispersion in the self-organizing dynamic mixture increases on increasing the molecular weight. Exfoliation ceases in a matrix with chains beyond a certain length. [1] R.B. Pandey and B.L. Farmer, J. Polym. Sci. Part B 46, 2696 (2008).

3This work is supported by AFRL.

S1.00008 Creating Janus Particles on Polymer Templates

MARLA MCCONNEL, University of Pennsylvania, MATTHEW KRAEUTLER, SHU YANG, RUSSELL COMPOSTO, University of Pennsylvania — Gold nanoparticles and their unique optical properties have been the topic of many recent research efforts. These optical properties are associated with the collective oscillations of conduction band electrons, and can be tuned in the visible range by changing the size and shape of the particles. In this study, we assembled spherical gold nanoparticles (13 nm in diameter) on spherical amine-modified silica particles (100 nm - 800 nm), which were covalently linked to a polymeric surface. Because gold has a strong affinity for amines, the modified silica particles served as an ideal template for assembling the gold nanoparticles. By varying the diameters of the silica particles, it is possible to tune the separation between the gold particles, resulting in a change in optical response. Once the gold nanoparticles are attached to the silica spheres, they can be sintered. This technique produces Janus particles, because the gold nanoparticles are localized to the top surface of the silica particles, due to shadowing.

S1.00009 Mechanical Properties of Organized Microcomposites Fabricated by Interference Lithography

SRIKANTH SINGAMANENI, SEHOON CHANG, Georgia Institute of Technology, JI-HYUN JANG, MIT, WHITNEY DAVIS, Georgia Institute of Technology, EDWIN THOMAS, MIT, VLADIMIR TSUKRUK, Georgia Institute of Technology, GIT/MIT COLLABORATION — We demonstrate that organized, porous, polymer microstructures with continuous open nanoscale pores and sub-micron spacings obtained via interference lithography can be successfully utilized in a highly non-traditional field of ordered microcomposites. Organized microcomposite structures are fabricated by employing two independent strategies, namely, capillary infiltration and in situ polymerization of the rubbery component into the porous glassy microframes. The mechanical properties and ultimate fracture behavior of the single microcomponents and microcomposite structures are investigated at different scale lengths. The ordered single and bi-component microstructures with high degree of control over the microscopic organization of the polymeric phases result in excellent mechanical properties. Combining hard and soft polymer components provides multifunctional materials and coatings with synergetic properties and is frequently utilized for design of advanced polymeric composites.

1supported by NSF

S1.00010 Diamond-shaped small-angle scattering and the deformation of fibrous textures

WENJIE WANG, University of Vermont, N. SANJEEVA MURTHY, Rutgers University — Small-angle x-ray scattering from materials with fibrous texture are typically characterized by diamond-shaped equatorial streaks. Single family of elongated voids aligned along the fiber axis modeled as ellipsoids with a certain orientation distribution yield a fan-like 2D pattern. The diamond-shaped patterns from fibers, such as polyesters, polyamide 6 and polyacrylonitrile, could not be explained with such single class of misoriented voids. Analysis of the orientation distribution and the isointensity contours suggest that there are at least two distinct entities that contribute to this equatorial scattering. Voids with larger cross section (~ 20 nm dia.), which are likely to be in the interfibrillar regions, give rise to low-q contours with smaller eccentricities and respond poorly to deformation. Entities with smaller cross section (~ 5 nm dia.), which are likely to be in the intrafibrillar regions, give rise to high-q contours with larger eccentricities and respond to deformation in the same way as crystalline domains. The scattering from these objects appear as two distinct families of elliptical contours with different eccentricities, and the observed diamond-shaped scattering results from the superposition of these two sets of contours.

1Supported by NSF grant DMR 0735242.
S1.00011 Thin Film Optical Measurements on a Low-bandgap Platinum-Acetylide Conjugated Polymer Developed for Use in Organic Solar Cells. ZAHA NASROLLAH, UFL, Dept Physics, JIANGUO MEI, KATSU OGAWA, YOUNG-GI KIM, UFL, chem Dept, NATHAN HESTON, UFL, chem dept, DANIEL ARENAS, UFL, phys Dept, TRACY MC CARLEY, LSU, chem dept, DAVID TANNER, UFL, phys dept, JOHN REYNOLDS, KIRK SCHANZIE, UFL, chem dept — An important barrier to overcome in producing high efficiency organic solar cells is to extend light harvesting capabilities into the near infrared. With strong absorption through the visible region and possible involvement of the triplet state in charge generation, Pt-acetylides have received recent attention as interesting and promising materials for photovoltaic applications. This presentation focuses on the thin film optical characterization of p-PBDT-Th. In order to obtain the absorption coefficient of this monomer, multiple lithography varied thicknesses were made and characterized by UV to NIR transmission and reflection measurements. We employed a thin film analysis using a Drude-Lorentz model to calculate the optical constants and to estimate the interference effects. From this model we were able to extract the absorption and extinction coefficients.

S1.00012 The study of polymer chain structure within macroporous polymer films by breath figure templating method. MINSU LEE, JUNG O. PARK, 1. School of Polymer, Textile and Fiber Engineering, 2. Center for Advanced Research on Optical Microscopy (CAROM), Georgia Institute of Technology, MOHAN SRI NIVASARAO1, 1. School of Polymer, Textile and Fiber Engineering, 2. Center for Advanced Research on Optical Microscopy (CAROM), — Macroporous films produced by breath figure templating methods have a microstructure with close packed and highly ordered pores. The water droplets condense from humid air flowing over a dilute polymer solution in a volatile solvent, due to evaporative cooling. Then, the water droplets closely pack over and sink into polymer solution. A close packed array of water droplets produces thin walls of polymer films where the polymer chains are confined. In our study, we have some evidence of the deformation of polymer chain within macroporous polymer films in areas where the polymer is confined. We will present our result on the deformation of polymer chain structure within polymer films.

S1.00013 Trimerization of Monocyanate ester in Nanopores. YOUNG PYO KOH, QINGXIU LI, SINDEE L. SIMON, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — Nanocostruction generally results not only in a Tg depression, but also in changes in reactivity. Recently, we showed that the polymerization reaction of bisphenol M dicyanate ester is enhanced in nanopores and that the Tg of the resulting polycyanurate product is depressed relative to the bulk. In order to examine the importance of an intracyclization side reaction, in this work we investigate the effect of nanocostruction on the reactivity and the Tg of a monocyancate ester and its cyanurate product. Due to the monofunctional nature of the reactant, there is no possibility for the intracyclization side reaction in this system. Using differential scanning calorimetry (DSC), we find the primary Tg decreases with decreasing pore size but the secondary (higher) Tg is independent of pore size. In addition, we find that the trimerization reaction rate increases as confinement pore size decreases, and in the 8 nm pores, the reactivity is accelerated by a factor of 20. The results are consistent with the Tg depression and accelerated reaction found previously for the nanoconfined difunctional reactant.

S1.00014 Diblock Copolymers under Nano-Confinement. DONG MENG, YUHUA YIN, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Nano-confinement strongly affects and can thus be used to control the self-assembled morphology of block copolymers. Understanding such effects is of both fundamental and practical interest. In this work, we use real-space self-consistent field calculations with high accuracy to study the self-assembled morphology of diblock copolymers (DBC) under nano-confinement for several systems, including 1D lamellae-forming DBC confined between two homogeneous and parallel surfaces, in nano-pores, and on topologically patterned substrates; 2D cylinder-forming DBC on chemically strip-patterned substrates; and 3D gyroid-forming DBC confined between two homogeneous and parallel surfaces. The stable phases are identified through free-energy comparison, and our SCF results are compared with available experiments and Monte Carlo simulations in each case.

S1.00015 First-Principles Prediction of Novel Technetium(IV) Halide Polymeric Compounds. PHILIPPE F. WECK, EUNJIA KIM, FREDERIC POINEAU, KENNETH R. Czerskewski, University of Nevada Las Vegas — We report the crystal structures of novel technetium tetrahalide polymeric compounds, TcX4 [X=F,Br,I], as predicted from first-principles calculations. Similar to TcCl4, TcF4 and TcBr4 compounds are orthorhombic with the centro-symmetric space group Pnma, while TcI4 crystallizes in the space group P21/c. The structures consist of distorted octahedral groups of composition TcX6 linked into endless linear chains. A possible explanation for the differences between these structures is offered in terms of varying degree of bonding within the polymeric chains.

S1.00016 Control self-assembled nanowire using chemically modified substrates. SHUSUKE ABURAYA, SATOSHI AKASAKA, MIKIHIITO TAKENAKA, HIROKAZU HASEGWAI, Kyoto University, YASUHIKO TADA, HIROSHI YOSHIDA, Hitachi Ltd, NIKOS HADJICHRISTIDIS, Athens University, KYOTO UNIVERSITY TEAM, HITACHI LTD TEAM, ATHENS UNIVERSITY TEAM — Block copolymer lithography is a promising method for fabricating periodical nanopatterns. Strongly segregated block copolymers are required for the formation of smaller size microphase-separated structures. In this study, we used a poly(styrene-b-dimethylsiloxane) (PS-b-PDMS) which has large Flory-Huggins interaction parameter. In addition, we investigated this cylinder-forming PS-b-PDMS has large segregation in the bulk condition by small-angle X-ray scattering (SAXS). Consequently, we demonstrated a fabrication of well-ordered arrays of 15nm period PDMS cylinder on the grating substrate with chemical modification. So, we can obtain less than 10 nm L/S fabrication.
S1.00018 Graphoepitaxy of 2D array of Spheres in Di-block Copolymers1, ADETUNJI ONIKOYI, EDWARD KRAMER, University of California, Santa Barbara — The use of block copolymer (BCP) thin films to create periodic structures on a nanolength scale has proved to be very effective [1-3]. However, removing defects and improving translational order in the periodic structures remain important goals. This study exploits a form of graphoepitaxy as a means to influence translational and orientational order in a poly(styrene-b-poly-2-vinylpyridine) (PS-b-PVP) diblock copolymer. Here, the domains of the BCP thin film are allowed to order within sub-micron sized wells of various shapes. Effects on order and 2D melting behavior are examined. The wells are patterned into silicon substrates using electron-beam lithography. Secondary ion mass spectroscopy and scanning force microscopy are then used to characterize the self-assembly process. Results show that a near perfect hexagonal 2D lattice can be obtained in diamond shaped wells of appropriate dimensions. Perfect 6 fold symmetry is disfavored in square wells; rather, regions of meta-stable square packing or defect dense regions of hexagonal packing are observed. Further studies are being performed to understand these effects on melting behavior. [1] Segalman et al. Phys. Rev. Lett., 2003, 91, 196101 [2] Kim et al. Nature, 2003, 424, 411 [3] Guarni et al. International Electron Devices Meeting

S1.00019 Stress-Strain Relation of Tire Rubber Consist of Entangled Polymers, Fillers and Crosslink, KATSUMI HAGITA, National Defense Academy of Japan, Y. BITO, Y. MINAGAWA, SRI, M. OMIYA, Hokkaido Univ., H. MORITA, UI, AIST, M. DOI, Univ. of Tokyo, H. TAKANO, Keio Univ. — We presented a preliminary result of large scale coarse-grained Molecular Dynamics simulation of filled polymer melts with Sulfor-crosslink under an uni-axial deformation by using the Kremer-Grest Model. The size of simulation box under periodic boundary conditions (PBC) is set to about 66 nm to consider length of entangled polymer chains, size and structure of fillers, and non-uniform distribution of crosslink. We put 640 polymer chains of 1024 particles and 32 fillers into the PBC box. Each filler consists of 1280 particles of the C_{2800} fullerene structure. A repulsive force from the center of the filler is applied to the particles. Here, the particles of the fillers are chosen to be the same as the particles of the polymers and the diameter of the filler is about 15 nm. The distribution of the fillers used in this simulation is provided by the result of 2d pattern RMC analysis for 2D-USAXS experiments at SPring-8. Sulfor crosslink is randomly distributed in the system. It is found that stress-strain curves estimated by applying a certain uni-axial deformation to the system in simulations are in good agreement with those in experiments. It is successful to show difference on the S-S curve between existence / absence of fillers and qualitative difference of attractive force between polymer and filler.

S1.00020 In situ Raman Spectroscopy Study of Stress Transfer between Carbon Nanotubes and Amorphous Polymer, MINFANG MU, Department of Materials Science and Engineering, University of Pennsylvania, SEBASTIAN OSSWALD, YURY GOGOSTI, Department of Materials Science and Engineering, Drexel University, KAREN WINNEY, Department of Materials Science and Engineering, University of Pennsylvania — Stress transfer mechanism in single wall carbon nanotube (SWCNT) / poly(methyl methacrylate) nanocomposites was investigated using Raman spectroscopy on composite fibers. Without specific SWCNT-polymer interactions, the effective stress transfer to SWCNTs is limited to a small strain regime (< 0.5%). At higher strain, the stress on SWCNTs decreases due to debonding at the nanotube-polymer interface. Debonding was also evident by scanning electron microscopy on fracture fiber surfaces produced by tensile testing. Overall, the presence of SWCNTs in composite fibers greatly improves their mechanical properties by two ways: a sufficient stress transfer at SWCNT-polymer interface and a SWCNT-induced polymer chain orientation. It was also observed that polymer chains transfer stress more effectively, and we attribute this to a greater extent of nanotube-polymer chain entanglement.

S1.00021 MD simulations of nanofibers, ROBERT LIVERPOOL, JOSEPH ORTIZ, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University — We use MD simulations to study the strength of polymeric nanofibers. The simulations will examine the role of chain orientation, internal stresses and surface effects on the modulus of nanofibers. The simulations are performed at above and below the glass transition temperature of the polymer. We also examine the effect of inclusions in the fiber on the modulus.

S1.00022 Structure, Dynamics, Loading Capacity, and Volume Phase Transition of Polymer Nanoparticles, KIRIL STRELETZKY, JOHN MCKENNA, IMAAN BENMERZOUGA, PUBLUDU PEIRIS, MEKKI BAYACHOU, Cleveland State University — Microparticles were synthesized in aqueous solutions of neutral polymer hydroxypropylcellulose (HPC) through self-association of amorphophilic HPC molecules and subsequent cross-linking. Dynamic Light Scattering (DLS) was used to study the transport properties of HPC microparticles below and above the volume phase transition. Highly non-exponential, multimodal microgel spectra were observed and successfully analyzed by spectral time moment analysis. The structure and dynamics of microparticles was found to depend on polymer and salt concentration, crosslinking density, solution temperature, and the rate of heating. HPC microparticles undergo a reversible volume phase transition in which microparticle volume swells/deswells by as much as a factor of thirty. The study revealed that higher polymer concentration results in smaller microparticles with lower shrinking capacity. The effective cross-linking density that yields relatively monodisperse microparticles was determined. The angular dependence of scattering demonstrated that microparticles are largely spherical particles though sometimes two different particle sizes are present. Finally, flow-injection amperometry was used to evaluate the loading capacity of microparticles. Preliminary results show the moderate injection agent uptake that varies with temperature dependent size of particles.

S1.00023 Cleavage Energies of Modified Layered Silicates by Molecular Dynamics Simulation, YAO-TSUNG FU, HENDRIK HEINZ, Department of Polymer Engineering, University of Akron — The cleavage energy of organically modified layered silicates indicates the thermodynamic propensity of exfoliation in polymer matrices. We find substantial cleavage energy differences upon variation in cation exchange conditions (PBC) is set to about 66 nm to consider length of entangled polymer chains, size and structure of fillers, and non-uniform distribution of crosslink. Dynamic Light Scattering (DLS) was used to study the transport properties of HPC microparticles below and above the volume phase transition. Highly non-exponential, multimodal microgel spectra were observed and successfully analyzed by spectral time moment analysis. The structure and dynamics of microparticles was found to depend on polymer and salt concentration, crosslinking density, solution temperature, and the rate of heating. HPC microparticles undergo a reversible volume phase transition in which microparticle volume swells/deswells by as much as a factor of thirty. The study revealed that higher polymer concentration results in smaller microparticles with lower shrinking capacity. The effective cross-linking density that yields relatively monodisperse microparticles was determined. The angular dependence of scattering demonstrated that microparticles are largely spherical particles though sometimes two different particle sizes are present. Finally, flow-injection amperometry was used to evaluate the loading capacity of microparticles. Preliminary results show the moderate injection agent uptake that varies with temperature dependent size of particles.

S1.00024 Large-scale nanocomposites simulations using hybrid particle/SCFT simulations1, SCOTT SIDES, Tech-X Research — Preliminary results from 2D simulations of block copolymer nanocomposites (Phys. Rev. Lett. Vol 96, 250601 (2006) have been performed using a hybrid self-consistent field theory (SCFT) algorithm. While these simulation results showed that the presence of nanoparticles could induce changes in block copolymer morphologies, quantitative agreement with experiments for the particle densities at this transition is not yet possible. A feature missing in the 2D hybrid simulations is the packing behavior of real three-dimensional spherical particles embedded in lamellar layers or hexagonally packed cylinders formed by linear diblock chains. In order to carry out these hybrid particle/SCFT 3D simulations a new object-oriented SCFT framework has been developed. The object-oriented design enables the hybrid/SCFT simulations to be performed in a framework that is both numerically efficient and sufficiently flexible to incorporate new SCFT models easily. In particular, this new framework will be used to investigate the distribution of particle positions in diblock lamellar layers as function of nanoparticle density to study the interplay of patterning due to diblock domain structure and the chain depletion interaction between spherical particles.

1Acknowledgements: National Science Foundation

1Supported by a subcontract from ORNL
were incorporated. First, 40 nm thick films of P(S-

After crosslinking the films, cylinder- or lamellar-forming BCPs were prepared without disturbing the underlying layers. For cylinder-

of glass transition in polymer films is still controversially discussed. For different experimental probes different dependencies are observed

In several cases a direct comparison with results from other dynamic methods like dielectric spectroscopy is

due to this reconstruction, the coating demonstrates low adhesion to hydrophilic, hydrophobic, and amphiphilic materials in both

at constant frequency nor for the traces in the activation diagrams.

suggested. Calculation systems based on neutral, doubly charged, and highly charged oligomers whose all ring are linked to have linear chains were

was preferred in industry for its simplicity and cost-effectiveness. To obtain high quality multilayer films with excellent durability, the compensation films must

the C-C path of neutral, dicationic, and dianionic oligomers, were investigated. Calculations were performed on systems containing 16 monomers, by using

trans-polyacetylene can be made electrically conducting by means of doping[1] several different conjugated polymers with interesting properties in the conducting

of neutral oligomers substituted by dimethyl and dimethylen. To estimate the electronic structures, the difference between corresponding bond lengths along

been well characterized. Calculation systems based on neutral, doubly charged, and highly charged oligomers whose all ring are linked to have linear chains were studied as model for the polaronic defects in doped polythiophenes. The energetics of the aromatic and quinoid structures is investigated using the both ends of neutral oligomers substituted by dimethyl and dimethylen. To estimate the electronic structures, the difference between corresponding bond lengths along

developments in the field of calorimetry which overcome these limitations. We set up a differential AC-chip calorimeter capable to measure the glass transition

on a lattice. We use a method that allows us to calculate the exact mean velocity of a particle for Monte-Carlo simulations to first reproduce the experimental results presented above. We then investigate different signals (e.g., telegraph signal) to determine the optimal conditions. Optimal conditions can be either higher velocities or larger velocity differences between particles.


trans-polyacetylene random copolymers and thus the perpendicular orientation of lamellae was achieved. The detailed

Elements provided by Eastman Chemical and Akron Polymer Systems and funding from Ohio Dept. of Development

Fabrication of Nanostructured Multilayers from Crosslinkable Block Copolymers

Fabrication of Nanostructured Thin Films which Adapt Low Adhesive Properties in Changing Environment

Hybrid nanostructured thin films which adapt low adhesive properties in changing environment

Glass transition in ultra thin polymeric films measured by differential AC-Chip calorimetry

S1.00025 DNA Electrophoresis: how partially denatured DNA stops moving in a gel. DAVID SEAN, GARY SLATER, University of Ottawa — During temperature gradient gel electrophoresis (TGGE), a DNA strand travels in a gel with a temperature gradient. As the strand travels in a position of higher temperature, the stability of the double helix is reduced resulting in melted domains. It has been experimentally observed that in a gel, a partially melted DNA strand exhibits a steep reduction in mobility — perhaps even trapping. The sequence dependent melting of DNA can therefore be translated into a sequence dependent position at which the strand appears to stop. Thus, this can be used as an effective method for discriminating between strands that differ only in composition. However, the dominant blocking mechanisms remain unclear. Blocking/trapping events are re-created using Langevin dynamics simulations using the ESPResSo package to understand the physics behind the observed steep reduction in electrophoretic mobility. From these simulations a relation between gel parameters and the mobility of the strand is proposed.

S1.00026 Detrapping Particles in a Gel: A Numerical Study ANTOINE DUBÉ, FRANCIS TORRES, GARY W. SLATER, University of Ottawa — Pulsed fields are widely used in gel electrophoretic separations to increase resolution. For instance, Boyde & To [1] presented experimental results for the separation of spherical particles using pulsed fields. They first used alternating fields of fixed amplitudes $(E_{max} = \pm |E|)$ applied in the forward direction for a duration twice as long as in the backward direction. They then used field interruption in order to allow particles to thermally detrap. In both cases, they reported that using a pulsed field makes the particles migrate faster. We model the gel used in electrophoresis as a 2D system of obstacles on a lattice. We use a method that allows us to calculate the exact mean velocity of a particle for Monte-Carlo simulations to first reproduce the experimental results presented above. We then investigate solutions signals (e.g., telegraph signal) to determine the optimal conditions. Optimal conditions can be either higher velocities or larger velocity differences between particles.


S1.00027 Electronic Structure of Aromatic and Quinoidic Oligothiophenes by First-principles Calculations HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University — Since the discovery in 1977 that trans-polyacetylene can be made electrically conducting by means of doping[1] several different conjugated polymers with interesting properties in the conducting and semiconducting phases have been discovered. Polyythiophene has a typical π-conjugated system, then many polythiophenes are synthesized and several have been well characterized. Calculation systems based on neutral, doubly charged, and highly charged oligomers whose all ring are linked to have linear chains were studied as model for the polaronic defects in doped polythiophenes. The energetics of the aromatic and quinoid structures is investigated using the both ends of neutral oligomers substituted by dimethyl and dimethylen. To estimate the electronic structures, the difference between corresponding bond lengths along

S1.00028 Probing Interfaces of Multilayer Polymeric Compensation Films for Liquid Crystal Display system WUMIN YU, MARK FOSTER, The University of Akron — Highly anisotropic polymer films formed by rigid-rod like aromatic polyimides show uniaxial negative birefringence and can be used as compensation films to widen the viewing angles of liquid crystal display system (LCD). Fluorinated pendent groups have been introduced to polyimide molecules to improve their solubility in common organic solvents. A new procedure for incorporating the compensation film in the multilayer LCD assembly by directly casting the polyimide film on a LCD unit as a substrate film, e.g. triaceteate cellulose (TAC), is preferred in industry for its simplicity and cost-effectiveness. To obtain high quality multilayer films with excellent durability, the compensation films must adhere well to the TAC substrates. X-ray and neutron reflectivity techniques are being used to determine how the interface width between the polyimide film and TAC substrate varies with changes in polyimide chemistry or casting process parameters.

S1.00029 Fabrication of Nanostructured Multilayers from Crosslinkable Block Copolymers DONGJUNE HWANG, EUNHYE KIM, HYUNJUNG JUNG, DU YEOL RYU, JOONA BANG, DEPT. OF CHEMICAL & BIOLOGICAL ENG., KOREA UNIV., KOREA TEAM, DEPT. OF CHEMICAL ENG., YONSEI UNIV., KOREA TEAM — In this work, we fabricated three dimensional nanotemplates using crosslinkable block copolymers (BCPs). We synthesized crosslinkable BCP, P(S-r-(N3)3-b)-PMMA, in which 1.5 mol % of crosslinkable azide (N3) groups were incorporated. First, 40 nm thick films of P(S-r-(N3)3-b)-PMMA, exhibiting the hexagonal arrays of perpendicularly oriented cylinders, were prepared on the silicon substrates. After crosslinking the films, cylinder- or lamellar-forming BCPs were prepared without disturbing the underlying layers. For cylinder-forming BCPs, it was observed that the cylindrical microdomains in respective layers were exactly registered. For lamellar-forming BCPs, the underlying layers could neutralize the interfacial interactions as PS-r-PMMA random copolymers and thus the perpendicular orientation of lamellae was achieved. The detailed structures of nanostructured multilayers were characterized by atomic force microscope (AFM) and scanning electron microscope (SEM), and grazing-incidence small-angle x-ray scattering (GISAXS).

S1.00030 Hybrid nanostructured thin films which adapt low adhesive properties in changing environment SERGIY MINKO, ROMAN SHEPAROVYCH, Clarkson University — We describe a nanostructured composite coating constituted of surface-grafted hydrophobic nanoparticles embedded in a hydrophilic, polyethylene oxide molecular brush. The responsive coating undergoes reconstruction from the morphology of rigid hydrophobic asperities, which hide the collapsed polymer brush in air, to the morphology of a hydrophilic brush-like layer engulfing the nanoparticles underwater. Due to this reconstruction, the coating demonstrates low adhesion to hydrophobic, hydrophobic, and amphiphilic materials in both dry and wet environments. The key property of the designed layer is the size of the nanoparticles that is bigger than the collapsed in air and smaller than the stretched in water polymer coil in the brush. This finding provides useful guidelines for the development of low-adhesive surfaces of materials.

S1.00031 Glass transition in ultra thin polymeric films measured by differential AC-Chip calorimetry H. HUTH, University Rostock, Inst. of Physics, Universitätplatz 3, 18051 Rostock, Germany, D.S. ZHOU, Dept. of Polymer Science and Eng., Nanjing University, Nanjing, 210093, China, C. SCHICK, University Rostock, Inst. of Physics, Universitätplatz 3, 18051 Rostock, Germany — The film thickness dependency of glass transition in polymer films is still controversially discussed. For different experimental probes different dependencies are observed and a generally accepted link to molecular mobility is not yet established. Calorimetry has proven to provide useful information about glass transition, because it establishes a direct link to energetic characterization. In several cases a direct comparison with results from other dynamic methods like dielectric spectroscopy is possible giving further insights. For thin films in the m... nm range standard calorimetric methods are mostly not applicable. In the recent years there are new developments in the field of calorimetry which overcome these limitations. We set up a differential AC-chip calorimeter capable to measure the glass transition in nanometer thin films with pJ/K sensitivity. Changes in heat capacity can be measured for sample masses below one nanogram as needed for the study of the glass transition in nanometer thin polymeric films. No thickness dependency of the glass transition temperature was observed within the error limits — neither at constant frequency nor for the traces in the activation diagrams.
S1.00032 Well-defined branched polymers for studying surface segregation\(^1\), BOXI LIU, SHIH-FAN WANG, RODERIC QUIRK, MARK FOSTER, University of Akron — A linear response theory by Wu et al. \(^1\) predicts that the surface segregation of a long-chain branched polymer blended with a linear polymer depends only on the type and number of chain ends or branch points in the linear and branched chains. Our previous neutron reflectivity results suggest that further details of the branching may impact the surface segregation. To better understand the roles of molecular architecture a new set of well defined branched polystyrenes have been synthesized by anionic polymerization. These molecules include a series of 6-arm pom-pom polymers with the same overall number of repeating units, chain ends and branch points, but varying length of central linear portion; a 6-arm star polymer constructed to be a better analog with 6-arm pom-pom polymers; and a deuterated linear polymer more analogous to the branched polymers. Bulk viscosities of these polymers have been measured and their surface segregation is being studied by neutron reflectivity. Reference: 1 Wu, D.T.; Fredrickson, G. H. Macromolecules, 1996, 29, 7919.

\(^1\)Acknowledgement: Funding provided by NSF: CBET 070730692

S1.00033 “Smart” Surfaces of Polymer Brushes , QIANG WANG, DONG MENG, Department of Chemical and Biological Engineering, Colorado State University — “Smart” surfaces, also known as stimuli-responsive surfaces, can change their properties (e.g., wettability, adhesion, friction, elasticity, and biocompatibility) in response to external stimuli (e.g., temperature, pressure, light, solvent selectivity, ionic strength, type of salt, pH, applied electric field, etc.). In this work, we use numerical self-consistent field calculations to study in detail the structure and stimuli- responses of various polymer brushes, including (1) the thermo- response of PNIPAM brushes in water, (2) solvent-response of uncharged diblock copolymer brushes, and (3) the stimuli- response of charged two-component polymer brushes (including both the binary A/B brushes and diblock copolymer A-B brushes) to ionic strength, pH, and applied electric field. Among the many design parameters (e.g., chain lengths, grafting densities, A-B incompatibility, degree of ionization of charged polymers, etc.) we identify those that strongly affect the surface switchability. Such knowledge is useful to the experimental design of these smart polymer brushes for their applications.

S1.00034 Adsorption of phospholipid bilayers onto pullulan-modified cellulose surfaces , HEEJUN CHOI, ZELIN LIU, ALAN ESKER, Virginia Tech — 1,2-Dimyristoyl-sn-glycero-3-phosphocholine (DMPC) vesicle adsorption onto regenerated cellulose and pullulan 4-bromocinnamate (P4BC) modified cellulose surfaces was investigated via surface plasmon resonance (SPR) spectroscopy and quartz crystal microbalance with dissipation monitoring (QCM-D). P4BC with a degree of substitution (DS) of 0.061 ± 0.002 from UV measurements and 0.058 from \(^1\)H NMR was synthesized from pullulan and 4-bromocinnamic acid to yield P4BC. The deduced thicknesses from SPR for DMPC layers were ~3.7 nm (bilayer) on regenerated cellulose surfaces and ~2.1 nm (monolayer) on P4BC modified cellulose surfaces. Qualitative analysis of the QCM-D data also indicated that the DMPC layers on P4BC modified cellulose surfaces were thinner than on regenerated cellulose surfaces.

S1.00035 Robust Self-Assembly of Highly Ordered Complex Structures by Controlled Evaporation of Confined Microfluids , ZHIQUN LIN, MYUNGHWAN BYUN, SUCK WON HONG, Iowa State University — We demonstrate a robust, one-step method of evaporating polymer solutions in curve-on-flat geometries to create versatile, highly regular microstructures in a precisely controlled environment, as well as offering a comprehensive study of the influence of different upper surfaces on complex structure formation via controlled evaporation. Our method further enhances current fabrication approaches to creating highly ordered structures in a simple and cost-effective manner, with the potential to be tailored for use in photonics, electronics, optoelectronics, microfluidic devices, nanotechnology, and biotechnology.

S1.00036 A new class of bio-heat resisted polymer blend . , SEONGCHAN PACK, TAKASHI KASHIWAGI, TADANORI KOGA, MIRIAM RAFAILOVICH — Increasing in oil prices and environmental concerns is a driving force to seek out alternative materials. A completely biodegradable starch is a candidate for the alternative materials. Since the starch is brittle, it must be mixed with other polymers. In order to make a thermoplastic starch (TPS), we need a bio-compatibilizer to increase a degree of compatibilization. The biocompatibilizer can be a small molecules or nanoparticles with the small molecules, which leads to improved material properties. In order to demonstrate a possible biocompatibilizer, we first developed a corn-based starch impregnated with non-halogenated flame retardant retardants. The starch was blended with Ecoflex®, a biodegradable polymer. Using SAXS and USAXS we characterized structures of the compounds with different amount of Ecoflex® by weight. Furthermore, the addition of 5% nanoparticles in the compounds increased the Young’s Modulus and impact toughness significantly. The compounds also did flame test. It is indicated that the compound with the addition of the nanoparticles would pass with a UL-94V0 rating. Therefore, the procedure for producing these TPS compounds can be applied to any biodegradable polymers, manufacturing a new bio-heat resisted compound.

S1.00037 Controlled morphology of biodegradable polymer blends , SASIWIMON BUDDHIRANON, THEIN KYU, The University of Akron — Phase diagrams of biodegradable polymer blends containing poly(ε-caprolactone) (PCL) and poly(d,l-lactic acid) (PDLLA) having two different molecular weights were established by means of cloud point measurement and differential scanning calorimetry. Subsequently, the theoretical phase diagram was calculated self-consistently based on the combination of Flory-Huggins free energy for liquid-liquid phase separation and phase field free energy for crystal solidification. The phase diagrams thus obtained were LCST type or hour-glass type, which depended on molecular weight of PDLLA utilized. Guided by the phase diagram, the emerged morphology was determined as a function of blend concentration and temperature. It appears that the morphology control is feasible that ultimately affects the end-use property of PCL/PDLLA blends. A wide variety of morphology of biodegradable polymer may be developed with the porous structure and pore size to control scaffold porosity and the rate of drug delivery.

S1.00038 A Spectroscopic Investigation on the Structural Evolution of Soy Based Polyurethane Foams , DEEPA PUTHANPAREMBIL, CASEY KIMBALL, SHAW L. HSU, University of Massachusetts Amherst — Our current research deals with an economical and renewable soy based polyol for use in polyurethane foams. Infrared spectroscopic studies have revealed that the amount of polyurea segments formed and the kinetics of their formation in soy based polyurethane foam systems are considerably different from traditional systems employing ethylene oxide – propylene oxide based polyols. The most crucial aspect of this research is the miscibility of water in the reactive mixtures involving extremely hydrophobic soy-based polyols. High Field Nuclear Magnetic Resonance Spectroscopy (NMR) with D₂O as the probing agent was employed to determine the miscibility behavior at the molecular level. This technique was able to establish the structure and location of dispersed water, which can be extremely different based on the polyols used, thus affecting the morphology of the foam. The length and amount of polyureas directly impact the kinetics of the phase separation process to form the hard-segment rich domains and associated physical properties. The aggregation of these polyurea hard domains was characterized by the hydrogen bonds formed. This structural transformation as a function of reaction is also reflected in the segmental relaxation kinetics characterized by spin-spin diffusion, measured using a low field NMR instrument.
S1.00039 Evaporative Organization of Hierarchically Structured Polymer Blend Rings, MYUNG-WAN BYUN, SUCK WON HONG, Iowa State University, FENG QIU, The Key Laboratory of Molecular Engineering of Polymers at Fudan University, Shanghai, China, ZHIQUN LIN, Iowa State University — We report the first study of the controlled, evaporative self-organization of a polymer blend from a sphere-on-flat geometry. In this study, a drop of polystyrene (PS) and poly(methyl methacrylate) (PMMA) toluene solution evaporated in the sphere-on-flat geometry. The combination of controlled, consecutive pinning-depinning cycles (i.e., “stick-slip”) of the contact line at the edge of the geometry, spontaneous phase separation of incompatible polymers at the microscopic scale, and a dewetting process in the late stage of phase segregation led to the formation of gradient, hierarchically structured polymer blend rings composed of phase-separated PS and PMMA. This facile approach offers a new way of simultaneously processing two or more nonvolatile components via controlled evaporation to produce new kinds of structures with hierarchical order in a simple, robust, and one-step manner.

S1.00040 Directing Hierarchical Assembly of Block Copolymer-Based Supramolecules Using Small Molecule Blends, PAUL TILLBERG, MATTHEW RICHARDS, TING XU, Dept. of Materials Science and Engineering, UC Berkeley — Block copolymer-based supramolecules can be obtained by selectively hydrogen-bonding amphiphilic small molecules to one block of a diblock copolymer. Through interactions between small molecules and the polymer backbone and between separate polymer blocks, hierarchical self-assembled structures are achieved on length scales unavailable through traditional top-down engineering methods. We aim to introduce an additional independent design parameter by hydrogen-bonding a mixture of small molecules to the polymer backbone. The phase behavior of the small molecules can be tailored to obtain an extra level of molecular control and generate novel hierarchical structures within block copolymer domains. Ultimately, this principle can be used to generate tri- or multi-block copolymer behavior by hydrogen-bonding different small molecules to simple homo or diblock copolymers. We will present preliminary data obtained by adding fluorinated alkyl phenols to the model block copolymer-based supramolecular system consisting of polystyrene-block-poly(4-vinylpyridine) with alkyl phenols hydrogen-bonded to pyridine groups.

S1.00041 Chirality Effect on Flory-Huggins Interaction Parameters in Polylactate-b-Poly(ethylene-co-1-butene)-b-Polyether Tricblock Copolymers, WEIQIANG CAO, LEI ZHU, Polym. Program, Inst. of Mater. Sci. and Dept. of Chem., Mater. and Biomolecular Eng., University of Connecticut, Storrs, CT 06269-3136, LIXIA RONG, BENJAMIN S. HSIAO, Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400 — In this work, a set of well-defined polylactide-b-poly(ethylene-co-1-butene)-b-polyether (PLA-PEB-PLA) tricblock copolymers were synthesized by controlled ring-opening polymerization of corresponding lactide monomers (L-lactide and racemic mixture of D- and L-lactides) using Sn(Oct)2 as the catalyst. The volume fractions of PLA in the tricblock copolymers were adjusted by tuning its molecular weight. The mesophase morphology and phase transitions in these tricblock copolymers were studied by temperature-dependent small-angle X-ray scattering (SAXS). The Flory-Huggins interaction parameter $\chi$ between EB and lactide as a function of temperature were estimated from the order-disorder transition temperature ($T_{ODT}$) using the mean-field critical ($\chi_N$) values. The effects of PLA chirality on both Flory-Huggins interaction parameter and segmental lengths were investigated.

S1.00042 Structure of PEO-b-PPO-b-PEO Triblock Copolymer Inclusion Complexes with Beta-Cyclodextrin, CHI-CHUN TSAI, STEPHEN Z.D. CHENG, BERNARD LOTZ, JIN HUANG, YONGMING CHEN — Inclusion complexes, formed by non-covalent host-guest interactions, have been extensively investigated because they can be useful as building blocks for constructing supramolecular structures. Cyclodextrins (CDs), due to their good water-solubility and ability to include a wide range of guest molecules, have been the most intensively studied host molecules. CDs are shaped like a shallow truncated cone, with a hydrophilic outer surface as well as primary (narrower end) and secondary (wider end) hydroxy groups on the rim of the molecule. The cavity, which is constructed with alkyl groups and glycosidic oxygen atoms, is hydrophobic and can act as a host for a great variety of hydrophobic molecular guests. A series of host-guest inclusion complexes were prepared with beta-cyclodextrin (beta-CD) and PEO-PPO-PEO triblock copolymers of varying molecular weights and compositions. The middle PPO block of the copolymers can be selectively included by beta-CD to form an inclusion complex while the PEO blocks cannot. These inclusion complexes can further self-assembled into supramolecular structures in aqueous solution. The inclusion complexes and self-assembled supramolecular structures were characterized by Nuclear Magnetic Resonance, X-ray diffraction, and Differential Scanning Calorimetry experimental methods.

S1.00043 Order-to-Order Transitions of Block Copolymer in Film Geometry, CHANGHAK SHIN, HYUNJU AN, JUNE HUH, DU YEOL RYU, Yonsei University, Korea — The phase transition behavior for an asymmetric polystyrene-block-polyisoprene (PS-b-PI) in film geometry, like the order-to-order transition, was investigated by in-situ grazing incidence small angle x-ray scattering (GISAXS). Unlike the bulk behavior, the micromdomain (or lattice) orientations in film geometry are influenced by the weak interfacial interactions between the native oxide layer and the polystyrene block due to the efficient interconnectivity, while the random orientation is observed for lamellar (LAM) structure. Compared with the bulk phase behavior, temperature dependence on the morphology leads to the enhancement of LAM morphology, the shifts of transition temperatures for the others, because interactions at the substrate/polymer and polymer/air interfaces influence this free energy balance.

S1.00044 Interfacial Polarization and Field Induced Orientation in Self Assembled Nanostructured Soft Ion Conductors, THOMAS THURN-ALBRECHT, PETER KOHN, KLAUS SCHROTER, Martin-Luther-University Halle-Wittenberg, Germany — We report about the effects of interfacial polarization in and upon a self assembled nanostructured ion conductor, consisting of an ordered, lamellar block copolymer with a Lithium salt dissolved selectively in one component. Impedance spectroscopy in combination with frequency dependent orientation experiments enable a quantitative analysis of ionic polarization and a direct demonstration of its aligning effect on the interfaces. The transition time from the fast dielectric to the slow ionic interfacial polarization is much longer than expected from classical Maxwell-Wagner-Sillars theory and attributed to the formation of diffuse double layers at the internal interfaces. The much stronger orientation effect of ionic as compared to dielectric polarization offers a new route to align microdomains and therewith the ion conducting paths of the polymer.
S1.00045 FTIR Investigation of Ion Environments in PEO-based “Single Ion” Polymer Conductors

MINGFU LU, JAMES RUNT, PAUL PAINTER — The infrared and Raman spectra of ionomers and electrolytes containing sulfonate groups have been previously studied in great depth. If the cation - anion interaction is relatively strong, the doubly degenerate asymmetric SO3- stretching mode becomes split into two components, while the symmetric SO3- stretching mode displays bands that can be assigned to the “free” (solvated) anion, neutral pairs and aggregates. In this paper we investigate a series of PEO-based polyester copolymer ionomers, with sulfonate anions covalently bound to the polymer chains, using FTIR spectroscopy. Ion content is systematically varied by changing the ratio of ionic to non-ionic isophthalate groups while keeping a fixed PEO segment molecular weight of 600. In the FTIR spectra of these ionomers, a splitting of the asymmetric mode is observed and only a single symmetric stretching band characteristic of some form of aggregated structure is apparent. There is no evidence that “free” or solvated ions are present. In addition, various ethylene oxide modes of vibration are shifted in frequency in a similar manner to those observed in studies of complexes of known structure, indicating their involvement in the formation of the aggregate.

S1.00046 Origin of the low-q X-ray scattering behavior in poly(ethylene oxide)-based ionomers

AMANDA MCDERMOTT, GREGORY TUDRYN, Penn State University, JAN ILAVSKY, Argonne National Laboratory, ANDREW ALLEN, National Institute of Standards and Technology, RALPH COLBY, JAMES RUNT, Penn State University — Ultra-small-angle X-ray scattering is used to investigate a series of single-ion-conducting PEO-based polyester copolymers with varying amounts of ionic sulfonate groups covalently bound to the polymer chains. We observe a low-q scattering component found in many polymers, including the neutral version of our material, and generally attributed to impurities. However, both the intensity and power-law slope of this scattering intensity upturn increase at high ion contents, indicating that it contains structural information about intentionally added ions. We discuss the interpretation of this feature with insight from atomic emission spectrophotometry, a critical ion fluctuation model, and the X-ray scattering behavior observed with several different cations and a range of concentrations.

S1.00047 New type of Reverse Osmosis Membrane via Layer-by-Layer Assembly Process

JUNWOO PARK, JOONA BANG, JEONGJU PARK, JINHAN CHO, DEPARTMENT OF CHEMICAL & BIOLOGICAL ENGINEERING TEAM, SCHOOL OF ADVANCED MATERIALS ENGINEERING TEAM — As to the commercial RO membranes for desalination, the polyamide (PA) based membranes have been widely used so far. However, they still have limitations, such as low permeability, bio-fouling, etc. In this work, we propose new types of polyelectrolyte-membranes which can overcome such problems. The membranes were designed by layer-by-layer (LbL) method using polyelectrolytes, including poly(allylamine hydrochloride), poly(styrene sulfonate), poly(acrylic acid), etc. Individual layers were adjusted by pH condition and number of deposition. The resulting multi-layered membranes were crosslinked by heat to provide the good durability. The morphologies were characterized by FE-SEM and AFM and the salt rejection was monitored by ion chromatography. By optimizing the membrane structures, we found that the water permeability was enhanced, while the salt rejection was as efficient as RO membranes. We believe that these results can provide the new protocol to design the advanced RO membrane.

S1.00048 ABSTRACT WITHDRAWN —

S1.00049 Simultaneous Prediction of Upper and Lower Critical Temperatures in Polymer Solutions Using a Constant Parameter Set

ELIZABETH CLARK, JANE LIPSON, Dartmouth College — Polymer solutions commonly exhibit phase separation and so the ability to predict temperatures and compositions associated with immiscibility is advantageous to experimentalists. We have been applying a simple lattice model that is capable of capturing both upper (UCST) and lower critical solution temperature (LCST) type phase behavior for polymer blends. Most recently we have become interested in mixtures which simultaneously exhibit both types of phase behavior. Examples include polysisobutylene (PIB) in pure and mixed solvents, and cyclohexane/poly styrene mixtures. We have found that with a single set of temperature-independent parameters the lattice theory is capable of capturing all the physics of these solutions; in addition we discuss conditions under which ‘hourglass’ phase diagrams result.

S1.00050 Monte Carlo simulations to study the effect of static and dynamic properties of polymer melts

KIRAN KHANAL, JUTTA LUETTMER-STRATHMANN, Department of Physics, The University of Akron, Akron, Ohio — Static and dynamic properties of polymers are affected by the stiffness of the chains. In this work, we investigate structural and thermodynamic properties of a lattice model for semiflexible polymer chains. The model is an extension of Shaffer’s bond-fluctuation model and includes attractive interactions between monomers and an adjustable bending penalty that determines the Kuhn segment length. This allows us to model melts of flexible and semiflexible chains. For this work, we performed Monte Carlo simulations for polymer melts with a range of bending parameters and densities. Results for chain dimensions show that the Kuhn segment length increases monotonously with the bending penalty and has a linear dependence for a range of bending parameters. Results for self diffusion constants show that the translational mobility is strongly reduced by increasing chain stiffness. We also investigate the effect of chain stiffness on thermodynamic properties of the melts.

S1.00051 Scaling of dynamic properties of polymer melts using friction coefficients of phantom chains - A Monte Carlo simulation study

NENAD STOJILOVIC, John Carroll University, JUTTA LUETTMER-STRATHMANN, The University of Akron — A Monte Carlo simulation method is used to test two different models of athermal polymer melts. In one model chains are allowed to cross (phantom chains) whereas in the other bond crossing is forbidden (real chains). We confirmed that the conformational properties of both types of polymers are similar and analyzed the differences in chain dynamics due to entanglements of real chains. Phantom chains that are sufficiently long exhibit Rouse dynamics, so that friction coefficients can be extracted from self diffusion coefficients. For real chains, on the other hand, entanglement effects complicate the determination of friction coefficients. In this work, we use friction coefficients from phantom chains to investigate the scaling behavior of dynamic properties of real chains.
S1.00052 Tactility effects on viscoelastic properties of polystyrenes1. CHIEN-LIN HUANG, CHI WANG, Department of Chemical Engineering, National Cheng Kung University — Polystyrenes (PS) with a similar molecular weight and distribution but different tacticities, i.e. syndiotactic (s-PS), atactic (a-PS), and isotactic (i-PS), have been used in this study to show a comparison to reveal their differences in the viscoelastic properties. Our attention was focused on the influence of the PS tacticity on the rheological properties, especially the plateau shear modulus \( G'' \) and entanglement molecular weight \( M_e \). Based on the time-temperature superposition principle, the master curves of dynamic storage modulus \( G' (\omega) \), dynamic loss modulus \( G'' (\omega) \), and tan\( \delta \) at a reference temperature of 280°C were constructed. The feasibility of conventional approaches for determining \( G'' (\omega) \), i.e. minimum tan\( \delta \) criterion, the integration method, and an empirical equation derived by Wu, has been discussed and compared; the corresponding \( M_e \) is then derived by the classical relation: \( M_e = \rho R T / G'' \). Our results show that the measured \( M_e \) and activation energy for flow are similar for s-PS and a-PS, but the highest for i-PS. In addition, the zero shear viscosity of i-PS is ca. one order larger than that of s-PS and a-PS.

1Thanks for NSC financial support.

S1.00053 Stress-induced Mobility in Polymer Glasses During Multistep Creep Deformation. HAU-NAN LEE, KEEWOOK PAENG, STEPHEN SWALLEN, MARK EDGER, Department of Chemistry, University of Wisconsin-Madison, ROBERT RIG- GLEMAN, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison. An optical photobleaching experiment and molecular dynamics simulations have been used to study the changes in segmental dynamics of a polymer glass during uniaxial creep deformation. Both experiment and simulation observe that segmental mobility increases more than a factor of 100 during deformation. Both show a strong correlation between strain rate and mobility in single step creep. However, in multistep creep and recovery, the correlation between strain rate and mobility is broken in both experiment and simulation; this emphasizes that no simple mechanical variable universally exhibits a simple relationship with molecular mobility. Interestingly, in contradiction to the Eyring model, both experiments and simulations show an increase in segmental mobility immediately follows a significant drop in stress.

S1.00054 Unusual Spherulite Radial Growth Rate Kinetics of Poly(ethylene adipate): Observation of a Double Maximum in Growth Rate Curve. KATHY SINGFIELD, ASHLEY ROWE, Saint Mary’s University — Poly(ethylene adipate) (PEA) is an aliphatic polyester often blended in small amounts with aromatic polyesters in order to impart some of its biodegradability to the resultant blend. Hot-stage polarized-light microscopy and differential scanning calorimetry have been used to investigate the isothermal melt-crystallization kinetics and thermal behaviour of PEA. The unusual spherulite radial growth rate dependence on isothermal crystallization temperature exhibits two maxima. A change in spherulite morphology from banded to non-banded spherulites is associated with the phase behaviour anomaly. The results are interpreted in terms of traditional Hoffmann-Lauritzen growth kinetics.

S1.00055 Simultaneous Dielectric Spectroscopy and X-ray Diffraction of Poly(ethylene terephthalate) and PET/Carbon Nanotube Nanocomposites. BRET STENGER, LEI YU, PEGGY CEBE, Tufts University Department of Physics and Astronomy, CEBE RESEARCH GROUP TEAM — The crystallization of poly(ethylene terephthalate) (PET) and a nanocomposite of PET with multi-walled carbon nanotubes (MWCNTs) were studied by simultaneous wide and small angle X-ray diffraction and dielectric relaxation spectroscopy. Our purpose is to determine whether the MWCNTs affect the cold crystallization kinetics or phase structure of the PET host. The nanocomposites contained 2% MWCNT by weight, and were prepared by solution mixing, and then compression molding into film. Dielectric measurements were made at frequencies from 100 Hz to 1 MHz, in parallel plate geometry. Measurements of the samples during cold crystallization (T<100-120°C) were used to investigate the relationship between the growth of crystals and the restriction of the molecular mobility of the amorphous phase. In agreement with previous work, results indicate that a heterogeneous distribution of amorphous regions exists, implying both interlamellar and interfibrillar/interphersulitc placement of the amorphous chains. Addition of carbon nanotubes to the PET increased the rate of cold crystallization, but did not affect the glass transition relaxation process.

S1.00056 Crystallization kinetics and the orientation of crystals under cylindrical nanoconfinement. KYUNCHEE LEE, EUNTAEK WOO, KYONG WOOK NOH, School of Chem. and Bio. Eng., Seoul National University, YOUNG GYU JEONG, School of Adv. Mater. and Sys. Eng., Kumoh National Institute of Technology, JUNE HUH, School of Mater. Sci. and Eng., Seoul National University, KYUSOON SHIN*, School of Chem. and Bio. Eng., Seoul National University — Crystallization kinetics, together with crystal orientation, is affected by the imposed geometric constraint. We investigated that crystallization of polymer and metal in nanopores with the variation of pore diameter. Crystallization of PE in nanopores is dominated by nucleation and the crystal growth is restricted by the limited space. On the basis of classical nucleation theory, we found that homogeneous nucleation dominates in larger pores while heterogeneous nucleation governs in smaller pores. We also investigated the orientation of crystal structures of polymer and metal in cylindrical nanopores, and found that the crystal orientation is influenced by crystallization mechanism in nanoscopic cylindrical pores, the crystal growth is limited and the crystals are preferentially oriented along the pore axis.

S1.00057 Crystallization of Polyethylene on nucleating and on passive substrates. THOMAS HENZE, KLAUS SCHROETER, THOMAS THURN-ALBRECHT, Institute of Physics, Martin-Luther-University Halle-Wittenberg, D-06099 Halle, Germany — Since the late 1950’s it has been known that polymers are able to crystallize epitaxially on suitable crystalline substrates. Whereas epitaxial crystallization experiments have been typically performed from solution, we here present a study of the morphology of thin films of polyethylene crystallized from the melt on a number of substrates with different ability to invoke crystallization, namely mica, NaCl, SiO\(_2\) and HOPG. Using intermittent-contact mode AFM very different structures are observed on the surface of the polymer film depending on the kind of substrate as well as film thickness. For very thin films (~30 nm) on NaCl and HOPG edge on lamellae, oriented in domains according to the underlying crystal lattice, show up while for mica and SiO\(_2\) flat-on lamellae dominate. With increasing film thickness (up to 130 nm) the orientation of the lamellae on HOPG and NaCl becomes weaker, while on mica and SiO\(_2\) a spherulitic morphology develops, which is not present in the case of HOPG and NaCl.

S1.00058 Impact of Protein-Metal Ion Interactions on the Crystallization of Silk Fibroin Protein1. XIAO HU, QIANG LU, DAVID KAPLAN, PEGGY CEBE, Tufts University — Proteins can easily form bonds with a variety of metal ions, which provides many unique biological functions for the protein structures, and therefore controls the overall structural transformation of proteins. We use advanced analytical analysis methods such as temperature-modulated differential scanning calorimetry and quasi-isothermal TMDSC, combined with Fourier transform infrared spectroscopy, and scanning electron microscopy, to investigate the protein-metallic ion interactions in Bombyx mori silk fibroin proteins. Silk samples were mixed with different metal ions (Ca\(^{2+}\), K\(^+\), Na\(^+\), Cu\(^{2+}\), Mn\(^{2+}\)) with different mass ratios, and compared with the physical conditions in the silkworm gland. Results show that all metallic ions can directly affect the crystallization behavior and glass transition of silk fibroin. However, different ions tend to have different structural impact, including their role as plasticizer or anti-plasticizer. Detailed studies reveal important information allowing us better to understand the natural silk spinning and crystallization process.

1Research supported by the National Science Foundation, Polymers Program of the Division of Materials Research, through grant DMR-0402849.
S1.00059 Effects of configurational defects on structural evolution in Poly(vinylidene fluoride-hexafluoropropylene) copolymers. SURIYAKALA RAMALINGAM, SHAW L. HSU, University of Massachusetts, Amherst — Crystallization kinetics of various crystallizable segments in Poly(vinylidene fluoride-hexafluoropropylene) [P(VDF-HFP)] copolymers have been analyzed using thermal techniques. These analyses are supported by spectroscopic and diffraction techniques, which directly measure the presence or absence of specific chain conformations or crystalline forms. Crystallization is constrained due to random distribution of the noncrystallizable bulky comonomer (HFP) along the crystallizable linear PVDF chains. Since the crystallites of different size/VDF chain lengths have different melting temperatures, it is possible to obtain a fraction of each crystallizable segment by selecting the crystallization temperature at various points below melting temperature. This fractionation has been accomplished by following the Successive Self-Nucleation/Annealing (SSA) method. The chain distribution and configurational defects, introduced by HFP, have been evaluated and correlated to the multiple thermal transitions in P(VDF-HFP) copolymers. In addition, it is interesting to find that the thermal fractionation can induce the above|conformation in highly constrained P(VDF-HFP) copolymers.

S1.00060 Polymorphism Behaviors of Electrospin Poly(vinylidene fluoride) Nanofibers. ZHENXIN ZHONG, DARRELL RENEKER, The University of Akron — Poly(vinylidene fluoride) (PVDF) and its copolymers have drawn great attention in recent years due to their attractive electrical properties such as ferro-, piezo- and pyro-electricity. Depending on its processing, PVDF can exhibit five different polymorphs. Among them, the beta phase has the highest piezo-, pyro- and ferroelectric activities. Electrospinning was used to produce thin polymer fibers. The polymorphic behavior of electrospun PVDF fibers was observed. Long cylindrical PVDF specimens with cross-sections in the range of 10 nm to 1 micron was obtained by varying the electrosprining conditions. Almost pure beta phase was obtained in electrospun PVDF nanofibers. The morphology and internal structure of single PVDF electrospin nanofibers were studied by electron transmission microscopy.

S1.00061 Electrospin Buckling Coils. YU XIN, DARRELL RENEKER, The University of Akron — Electrosprining offers a useful way to produce fibers with micron and nanometer scale diameter. The present work deals with the buckling phenomenon characteristic of a jet impinging upon the surface of collector. A viscous jet may have either tensile or compressive forces along its axis. The periodic buckling that is often observed is attributed to the occurrence of compressive forces as the jet decreases at the collector. With the increase of axial compressive stresses along the jet, a jet with circular cross sections first buckles by formation of sharp folds, and then by formation of coils. The resulting buckling patterns include zigzag patterns and coils that which can be controlled by changing parameters, such as density, viscosity, conductivity, voltage, polymer concentration, distance and volumetric flow rate. Uniformly buckled polymer fibers can be made at a rate of one turn per microsecond. An experimental apparatus was built to continuously collect buckling coils of nylon 6, from a water surface, into a multilayer sheet. These small “springs” and sheets will be tested for mechanical properties needed in biomedical applications.

S1.00062 Hierarchical Structure on Nanofiber via Combination of Electrospinning and Polymer Crystallization. XI CHEN, Drexel University, BINGBING WANG, RUCHA SHAH, CHRISTOPHER LI — We report the formation of hierarchically ordered polymer nanofiber structures, named as nano fiber shish kebabs (NFSKs), by combining electrospinning and controlled polymer crystallization methods. Both poly caprolactone (PCL) and poly (ethylene oxide) (PEO) nanofibers were produced by electrospinning. These polymer nanofibers served as the shish and a secondary polymer (block copolymer) was decorated on the nanofiber in the form of single crystal lamellae by either an incubation (slow crystallization), or a solvent evaporation (fast crystallization) method. The structural parameters of the NFSK such as the fiber diameter, periods, the kebab size etc., were readily controlled by changing the electrosprining and crystallization conditions. This hierarchical architecture is of great technological interest because it provides a platform for incorporating different functionalities into nanoscale fiber fibers in an ordered fashion.

S1.00063 PP/POSS Nanocomposites: Characterization and Properties of Melt Spun Fibers. BYOUNG-JO LEE, SAYANTAN ROY, SADHAN JANA, University of Akron — It is known that molecules of polyhedral oligomeric silsesquixoxane (POSS) can self-assemble into spherical, fibrillar, or lamellar nanoparticles by bottom-up self assembly process during mixing with host polymers. This study capitalizes on such nanoparticle formation to increase the melt strength and tensile properties of polyolefin blown films and spun fibers. A novel method was developed whereby a sorbitol-type nucleating agent was used as dispersion aids for POSS. The nucleating agent also served as templates for self-assembly of POSS molecules into nanoparticles of 25-200 nm in diameter. A typical polypropylene formulation containing 0.3 wt% nucleating agent and 5-10 wt% POSS was spun into fibers with close to 70% reduction in diameter and 40-45% increase in modulus and 70-75% increase in yield strength compared to unfilled PP. An optimum concentration of POSS was identified.

The authors thank NSF for providing financial support through grant number CMMI-0727231 and Hybrid Plastics for partnership and assistance with the materials.

S1.00064 Affine deformation in polymer networks. ANINDITA BASU, QI WEN, PAUL JANMEY, ARJUN YODH, University of Pennsylvania, DEPT. OF PHYSICS AND ASTRONOMY, UNIVERSITY OF PENNSYLVANIA COLLABORATION, INSTITUTE FOR MEDICINE AND ENGINEERING, UNIVERSITY OF PENNSYLVANIA COLLABORATION — An affine deformation is one where a macroscopic deformation applied on a body is translated uniformly to the microscopic level. Much existing theory, ranging from simple rubber elasticity to non-linear elasticity in biological polymer networks, is based on the assumption that deformations are affine. We explore the validity of the affine assumption by embedding micron-sized fluorescent beads within model polymer networks and quantifying their displacements when the sample is put under shear deformation. We quantify the non-affine deformations as functions of polymer chain density, cross-link concentration and find our results to be in qualitative agreement with current theories of rubber elasticity.

S1.00065 Length and Structure Dependence of Electron Transport in Organic Molecules. SHASHI KARMA, GOVIND MALLICK, US Army Research Laboratory, HAIYING HE, RAVINDRA PANDEY, Michigan Tech University — The electron transport through organic molecules is affected by a number of structural parameters, such as the length, dihedral angle, rotation around a single-bond, symmetry and charge distribution of frontier molecular orbitals. In addition, in a molecule-solvent hybrid system, the chemistry and physics of the molecule-solvent interface plays an extremely important role on electron transport through organic molecules. In order to gain an enhanced understanding of the effects of length, geometry and solid-molecule interface we have investigated electron transport through n-conjugated molecules of increasing lengths in contact with Au substrate by non-equilibrium Green’s function method within ab initio molecular orbital theory, density functional theory and semi-empirical methods. The effects of rotation around a single bond, change in dihedral angle and the length of the molecule on the transport properties are investigated. The results suggest a complex dependence of electron transport on one-electron energy levels, spatial characteristics of the wave function and geometry of the molecules. Further, the local density of states and location of metal Fermi level are also found to affect electron transport characteristics in a metal-molecule hybrid system.

S1.00066 PHASE TRANSITIONS AND STRONGLY CORRELATED SYSTEMS —
S1.00067 Color change of Ruby investigated by Raman and UV-vis. SEAN BRECKLING, YING ZOU, SHISHIR RAY, LARRY BUROKER, SOMADITYA SEN, MARK WILLIAMSEN, PRASENJIT GUPTASARMA. University of Wisconsin-Milwaukee — The origin of a distinct red color in Ruby (Al2O3:Cr3+) continues to be a fundamental unsolved question [1]. We report the synthesis of a series of samples of 2% Cr2O3 by solid state reaction [2] at temperatures varying between 900° and 1300°C. We observe a visible change in color at every stage, from light green, to grey, and to pink, indicating progressive incorporation of Cr3+ ions into the Al2O3 lattice. We report further investigations of x-ray diffraction analysis, Raman and UV-visible spectroscopy, and correlate the observed color changes with the evolution of vibration modes of the cage around CrO6 and band-gap states resulting from Cr incorporation. We also plan to report results from single crystals grown using a floating zone. [1]J.M. Garcia-Lastra, M.T. Barriuso, J.A. Aramburu and M. Moreno, Phys. Rev. B 72(2005)113104 [2]L.W. Finger and R.M. Hazen, J. Appl. Phys. 49(1978)5823

S1.00068 ABSTRACT WITHDRAWN —

S1.00069 Scattering of the Transverse Acoustic Phonon by Polar Nanodomains in the Relaxor Ferroelectric KTa1−xNbO3 (KTN)1, JEAN TOULOUSE, EUGENE IOLIN, Lehigh University, Physics Department and Center for Advanced Materials, BERNARD HENNION, DANIEL PETITGRAND, LLB, CEA, Saclay France, ROSS ERWIN, NCNR, NIST — We show that, in relaxors, the transverse acoustic (TA) mode displays a particularly original behavior, due its coupling to the transverse optic (TO) mode as well as to the polarization P of the Polar Nano-Domains (PND) that are ubiquitous in these special ferroelectrics. A neutron scattering study of the TA phonon frequency and damping, and especially of their q dependence, reveals that the PNDs condense in the form of platelets. In the relaxor range of temperatures, in which elastic diffuse scattering is also observed, the TA mode is strongly scattered by the PNDs. We compare our results with those from thermal conductivity studies of inhomogeneous solids and similar neutron results obtained in other perovskite systems. We also present a theoretical model that describes the scattering mechanism specific to relaxors, the TA-P-T0 interaction, is shown to fit the acoustic data well and also provides an estimate of the TO mode frequency and damping.

1This work is supported by the US Department of Energy under grant DE-FG-06ER46318.

S1.00070 93Nb NMR investigation of the multiferroic system Ba3NbFe3Si3O14, LLOYD LUMATA, NHMFL/Physics, Florida State University, M.J.R. HOCH, H.D. ZHOU, J.S. BROOKS, P.L. KUHNS, A.P. REYES, C.R. WIEBE, NHMFL/Physics, FSU — We present 93Nb nuclear magnetic resonance spectroscopy and relaxation data on the new multiferroic system Ba3NbFe3Si3O14. The spin-lattice relaxation rate 1/T1 and spin-spin relaxation rate 1/T2 show a peak at 26 K accompanied by broadening of the NMR lineshapes, characteristic of Néel ordering. Salient features of 93Nb NMR lineshapes in the ordered phase and temperature-dependent 93Nb Knight shifts will be discussed in relation to the possible bulking or tilting of the NbO6 octahedra (caused by magnet-lattice coupling) around the transition.

1This work was supported in part by NSF DMR-0602859 and performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-084173, EIEG grant, by the State of Florida, and by the DOE.

S1.00071 Phase Diagram of Floating Zone grown Multiferroic SmMnO3 and Mn site substitutions, SOMADITYA SEN, LARRY BUROKER, YING ZOU, SHISHIR RAY, MARK WILIAMSEN, PRASENJIT GUPTASARMA2, Physics Dept., Univ. of Wisconsin, 1900 E Kenwood Blvd., Milwaukee, WI 53211, USA — SmMnO3, a member of a Rare Earth manganite series of current interest due to the observation of multiferroic magnetoelectric properties, anisotropy in magnetic properties and an unconventional “compensation temperature” ~8K possibly arising from antiparallel S-Mn exchange interactions. Of particular interest here is charge disproportionation of Mn, competing magnetic and orbital order, and the proximity to a metal-insulator transition [1]. We report detailed studies of a high-quality single crystal of SmMnO3 grown from a floating zone, and the result of Mn-site substitution by elements with multiple valence states and octahedral coordination. We discuss magnetization, crystal structure refinement, and dielectric spectroscopy in 0.3<T<300 Kelvin and 0<H<9 Tesla. [1] Kurbakov, et.al., A, Physics of the Solid State, 46 – 9 (2004) 1704

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S1.00072 Magnetic and Specific Heat Studies of Multiferroic Hexagonal DyMnO3, YING ZOU, SHISHIR RAY, SOMADITYA SEN, MARK WILLIAMSEN, PRASENJIT GUPTASARMA1, University of Wisconsin-Milwaukee, USA — Rare earth (R) manganites (RMnO3) are well known to exhibit novel magnetic and magnetoelectric multiferroic properties. Under normal conditions, R=La through Dy yields orthorhombic lattice symmetry, whereas R=Ho through Lu yields hexagonal lattices. We confirm however that DyMnO3 single crystals, when grown in Argon from a floating zone, have a hexagonal lattice structure [1]. We report further new results in the H-T phase diagram in the range 0.3-300K and 0-T Tesla. Specific heat measurements show two transitions at 4K and 63K in the absence of a magnetic field. dc-Magnetization shows a cusp at 4K, which we attribute to a Dy3+ spin ordering. Time-dependent relaxation and frequency dependent shifting in ac susceptibility reveals a spin-glass behavior at this temperature, possibly suggesting an incommensurate Dy magnetic structure. An interesting bifurcation occurs for the high temperature transition (T~63K) in ac susceptibility with increase in frequency of the ac field. [1] V.Y.Ivanov et al, Phys.Solid State, 48(2006)1726

1Corresponding author

S1.00073 Low Temperature Phase Transitions in Single Crystal Magnetoelectric GdMnO3, MARK WILLIAMSEN, SHISHIR RAY, SOMADITYA SEN, YING ZOU, PRASENJIT GUPTASARMA1, University of Wisconsin-Milwaukee — GdMnO3 is proposed to have a magnetic phase transition from paramagnet to incommensurate antiferromagnet at 43K, further ordering to canted antiferromagnet around 23K, followed by Gd magnetic ordering at 6.5K[1]. We present further studies of a large single crystal of orthorhombic GdMnO3 grown by us from a floating zone, revealing additional features at lower temperature. Dielectric spectroscopy measurements confirm these new features. We also report dc-magnetization, frequency dependent ac-magnetization 2-300K, and specific heat 0.4-300K in a variable magnetic field 0-9T, and propose additional features in the magnetoelectric phase diagram. [1]T. Kimura,Phys.Rev.B 71,224425(2005)

1corresponding author
S1.00074 Local structure studies of multiferroic RMn2O5 (R=Bi, Pr, Gd)1, G. FABBRIX, LNLS/IFGW-UNICAMP, Campinas, Brazil, N.E. MASSA, LANAIS EFO-CEQUINOR, UNLP, cc962, 1900 La Plata, Argentina, E. GRANADO, IFGW-UNICAMP/LNLS, Campina, Brazil, C.A. MACIEL, IF-UFPR, Curitiba, Brazil, J.A. SOUZA, CCNH-UFABC, Santo André, Brazil, J.A. ALONSO, M.J. MARTINEZ, CSIC-ICM-CSIC, Cantoblanco, E28049 Madrid, Spain, G.M. AZEVEDO, LNLS, Campinas, Brazil — EAXFS measurements from 20 K to 300K were used to investigate the local structure of multiferroic RMn2O5 (R = Bi, Pr, Gd, TM TC 40K) in transmission mode at the Mn K- and R L- edges in the XAFS2LNS beamline and analyzed using the IFEFFIT and FEFF codes. For BiMn2O5, Mn K-edge reveals very small temperature dependence of the Debye-Waller factor (DWF) and an Einstein temperature (ET) from Mn-O bonds of 675±22 K, suggesting that MnO polyhedra are rigid. We find structural distortions in the first coordination shell at the Bi L-edge associated to vibrational anomalies in the Bi-O bonds. The quantitative analysis gives a measure of such distortions to two very distinct values of DWT and ET (294±7K and 462±28K) for these bonds on first shell. Similar results will be discussed in terms of disorder induced non-Fermi liquid behavior, related to the spin dynamics of the ferromagnetic nano-domains coexisting with antiferromagnetically correlated systems in the region.

1We acknowledge CAPES and CNPq for financial support.

S1.00075 Magnetism and non-Fermi liquid behavior in a Na0.78CoO2 single crystal1, ALEXANDER FEHER, A. ZORKOVSKA, M. KAJINAKOVA, A. BARAN, Centre of Low Temp. Physics, P. J. Safarik Univ. and Inst. Exp. Physics SAS, Kosice, Slovakia, C. T. LIN, J.P. PENG, Max-Planck-Institute for Solid State Research, Stuttgart, Germany, J.S. XIA, L. YIN, M.W. MEISEL, NHMFL and Dept. Physics, Univ. Florida — In recent years, significant interest has been devoted to high Na-doped cobaltates, in which the competition between geometric frustration, strong electronic correlations, and magnetic interactions leads to disorder, either correlated or non-correlated, and a variety of quantum states with possible QPTs are expected. Specific heat down to 100 mK and the ac-susceptibility at several frequencies and temperatures, down to 40 mK and in fields up to 10 T, of a layered Na0.78Co2O single crystal have been measured. The results will be discussed in terms of disorder induced non-Fermi liquid behavior, related to the spin dynamics of the ferromagnetic nano-domains coexisting with antiferromagnetically correlated systems in the region.

S1.00076 Transport and Magnetic Properties of ErNi2B2C, W.C. LEE, Dept. of Physics, Sookmyung Women’s Univ. Seoul 140-742, Korea — We measured the magnetization M(H,T) and magnetoresistivity ρ(H,T) of ErNi2B2C single crystal for magnetic fields perpendicular and parallel to the c-axis and with the current along the c-axis low temperature regions. From the magnetoresistivity measurements with the current along c-axis, we constructed the H2(T) curves for magnetic fields perpendicular and parallel to the c-axis and those were compared for curves with the current perpendicular to the c-axis. Also we constructed a magnetic phase diagram only the magnetic field perpendicular to the c-axis. We determined the critical behavior and calculate key observables at the transition and in the associated quantum Griffiths phase. We also briefly discuss the cases of superohmic and subohmic dissipation.

S1.00077 Antisymmetric Exchange in Antiferromagnetic Materials of Rhombohedral Structures, ALEXANDER BAZHAN, P.L.Kapitza Institute for Physical Problems, RAS, Moscow, Russia — Carriers transferrings, determined by wave functions and energy levels of i j magnetic and oxygen ions, which are determined by rhombohedral oxygen crystal fields and their particularities, are in discussions for identification of antisymmetric, Dzyloshinskii-Moria exchange, and energy levels of i j magnetic and oxygen ions, which are determined by rhombohedral oxygen crystal fields and their particularities, are in discussions

S1.00078 Infinite-randomness quantum critical points induced by dissipation, CHETAN KOTABAGE, University of Florida — We develop a strong-disorder renormalization group to study quantum phase transitions with continuous O(N) symmetry order parameters under the influence of both quenched disorder and dissipation. For Ohmic dissipation, as realized in Hertz’ theory of the itinerant antiferromagnetic transition or in the superconductor-metal transition in nanowires, we find the transition to be governed by an exotic infinite-randomness fixed point in the same universality class as the (dissipationless) random transverse-field Ising model. We determine the critical behavior and calculate key observables at the transition and in the associated quantum Griffiths phase. We also briefly discuss the cases of superohmic and subohmic dissipation.

S1.00079 Phase-transition behavior of Selenium confined in periodic mesoporous silica: an x-ray scattering study, KIYANGMIN LI, CONGSHANG WAN, GANG CHEN, Ohio University — Confinement of semiconductors in nanoporous media provides a new approach to modify their physical properties such as electric conductivity, thermal conductivity, and phase transition temperatures. To understand the effect of nanoscale confinement on the melting behavior of selenium, we now conduct x-ray scattering experiments on selenium that are confined in periodic mesoporous silica (PMS). Hexagonal MCM-41 and SBA-15 with cylindrical pores (2 - 30 nm in diameter) are synthesized and utilized as the host matrix. Under synchrotron x-ray scattering, the core-shell system is determined. Wide-angle x-ray scattering experiments are used to measure the melting points of selenium confined in cylindrical pores of various widths. Relation between pore width and melting point of Se is established and compared with the Gibbs-Thomson theory. Our study provides fresh insights into the applicability of the Gibbs-Thomson theory to inorganic semiconductors confined in nanoporous media.

S1.00080 Critical exponents taking into account dynamic scaling for adsorption on small-size one-dimensional clusters, VLADIMIR UDODOV, ANDREY TASKIN, KATANOV KHAKAS STATE UNIVERSITY COLLABORATION — Adsorption on small-size one-dimensional clusters is investigated using the Monte Carlo method. The effect of temperature and system size variations on adsorption is studied. Critical coefficients of the correlation length and dynamic critical coefficient z are calculated taking into account the hypothesis of dynamic scaling. The results obtained demonstrate that non-equilibrium adsorption in nanosystems can occur in a much different fashion than in macrosystems.

S1.00081 Infinite Size Scaling of Melting in Two Dimensions, KEOLA WIERSCHEM, MARTECH & Department of Physics, Florida State University, EFSTRATIOS MANOUSARIS, MARTECH & Department of Physics, Florida State University and Department of Physics, University of Athens, Greece — The melting transition of a two-dimensional Lennard-Jones fluid is studied using classical Monte Carlo methods. Melting in two dimensions is expected to occur via a two-stage process, with separate transitions for translational and orientational order. The second moments of the translational and orientational order parameters are analyzed, and dimensionless quantities are constructed. According to finite size scaling theory, such quantities should be a function of the ratio of system size to the length of the appropriate order parameter. Using the theoretical temperature dependence of the correlation length, and the fact that the correlation length approaches infinity at the critical point, the two melting transitions may be determined.
S1.00082 Probability Density Function at the 3D Anderson Transition, ALBERTO RODRIGUEZ, LOUELLA J. VASQUEZ, RUDOLF ROEMER, Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry CV47AL, United Kingdom — The probability density function (PDF) for the wavefunction amplitudes is studied at the metal-insulator transition of the 3D Anderson model, for very large systems up to $L^3 = 240^3$. The implications of the multifractal nature of the state upon the PDF are presented in detail. A formal expression between the PDF and the singularity spectrum $f(\alpha)$ is given. The PDF can be easily used to carry out a numerical multifractal analysis and it appears as a valid alternative to the more usual approach based on the scaling law of the general inverse participation rations.

S1.00083 Quantum simulation of Fermi-Hubbard models in semiconductor quantum-dot arrays, NA YOUNG KIM, Stanford University, TIM BYRNES, National Institute of Informatics, KENICHIRO KUSUDO, National Institute of Informatics, YOSHIHIISA YAMAMOTO, Stanford University — We propose a solid-state quantum simulator device to investigate a Fermi-Hubbard model including long-ranged Coulomb interactions. The device consists of an array of coupled quantum dots in a GaAs-based two-dimensional electron gas system. We launch an artificial lattice potential electrostatically by applying DC voltage to a periodically patterned thin film on top of the two-dimensional electron gas system. We tune both two competing energy terms – Coulomb interaction energy and kinetic energy - and the density of electrons independently, which enables us to construct a Hubbard phase diagram via differential conductance measurements. We consider the case of high average trapped electron density where more than the first bands are occupied. In this case, high mobility is still preserved and the effects of the Hubbard model would not be masked by impurities or disorder. We believe that a metal-Mott insulator quantum phase transition and a $d$-wave superconducting phase are observable in our proposed device according to the estimates of Hubbard parameters.

1Also at University of Tokyo

S1.00084 GENERAL THEORY (THEORETICAL METHODS) —

S1.00085 Coexistence of phases in final one-dimensional systems, VLADIMIR UDOODO, IVAN NAUMOV — Within the framework of L.D. Landau (1908-1968) approach it is shown, that two-phase equilibrium is possible in linear macrosystems of the final size at low temperatures. At further duration of temperature two-phase equilibrium becomes unstable and the system passes in a single-phase state. These results remain in force and at the account of interaction of interphase borders with each other and with the ends of linear system. Following Landau [1] we shall consider the linear system made of alternating pieces of two various phases. Points of contact between various phases (interphase borders) we shall present as a weak solution. For linear system of the limited size $L \{L>>1\}$ at low temperatures a single-phase state is stable. The increase in temperature will lead to phase transition of the first order in a two-phase state. The original cascade of phase transitions of the first order, because of increase of quantity of interphase border of item will be observed actually. 1. L.D.Landau, E.M.Lifshits. Theoretical physics. Statistical physics. A part 1. 4 edition. Moscow (In Russian): the Science publisher, 1995.

S1.00086 Variational Ground State of the One Dimensional Bose-Hubbard Model, J.D. MANCINI, Kingsborough College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University, R.K. MURAWSKI, Drew University — Recently, Eichenberger and Baeriswyl [PRB 76, 180504R, (2007)] have introduced a novel variational ansatz to study the two dimensional Hubbard model. Their scheme involves choosing a trial ket which consists of an exponential operator constructed from the Hamiltonian which then operates on a mean field ground state $|\psi_0\rangle$. In this study, we wish to extend this ansatz by combining it with a second ansatz in which a variational basis is constructed by systematically taking derivatives with respect to a (variational) parameter. The model we will study is the one dimensional Bose-Hubbard Hamiltonian which is used to investigate the properties of interacting bosonic atoms in a one-dimensional optical lattice. The Hamiltonian is given by

$$H_{bh} = -J \sum_{i=1}^{M} (a_i^\dagger a_{i+1} + \text{h.c.}) + \frac{U}{2} \sum_{i=1}^{M} n_i (n_i - 1),$$

where $a_i^\dagger$ ($a_i$) creates a boson at the lowest level localized on the $i$-th site, $J$ is the hopping energy and $U > 0$ is the onsite repulsion. Our results are then compared with other approximation methods such as Hartree-Fock-Bogoliubov theories and the variational Bijl-Dingle-Jastrow method.

S1.00087 Variational Ground-State of the One-Dimensional Heisenberg Model, J.D. MANCINI, Kingsborough College of CUNY, V. FESSATIDIS, Fordham University, R.K. MURAWSKI, Drew University, W.J. MASSANO, SUNY Maritime, S.P. BOWEN, Chicago State University — We wish to study the ground state of a spin system described by the Heisenberg Hamiltonian

$$H = -\frac{1}{2} J \sum_{i=1}^{M} \left\{ 2 \left( \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z \right) \right\},$$

where $\sigma^\pm = \sigma_x \pm i \sigma_y$ and $J$ is the interaction strength. We choose as our trial ket $|\psi_0 (\lambda)\rangle = e^{\lambda \hat{S}} |\phi_0\rangle$ where $|\phi_0\rangle$ is chosen to be the ferromagnetic state with all spins aligned downward, and $\hat{S}$ is the operator $\hat{S} = \sum_i \sigma_i^z$ with $\lambda$ a variational parameter. We then construct our variational basis by systematically taking derivatives of $|\psi_0 (\lambda)\rangle$ with respect to $\lambda$: $|\psi_N (\lambda)\rangle = \partial^N \psi_0 (\lambda)$. The lowest eigenvalue of the Hamiltonian matrix $E_0 (\lambda)$ is then minimized with respect to $\lambda$. Comparisons are then made with other approximation schemes.

S1.00088 Variational Moments Expansion, R.K. MURAWSKI, Drew University, J. MIKALOPAS, J.D. MANCINI, Kingsborough College of CUNY, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University — A number of years ago, a generalized moments expansion, GMX$(n, n)$ was derived as a novel way to calculate ground state energies of many body systems [PLA 349, 320 (2006)]. This scheme was based on a theorem by Horn and Weinstein for the "t-expansion" and was shown to be a generalization of an earlier connected moments expansion CMX, in which $\text{CMX} = \text{GMX} (1, 1)$. Here we wish to extend the GMX method, which involves matrix elements of moments of the Hamiltonian, to include a recent variational ansatz in which a variational basis is constructed by taking successive derivatives with respect to a (variational) parameter $\lambda$ that is introduced in a trial ket. The GMX expression for the ground state, $E_0 (\lambda)$ is then minimized within a given subspace of the Hilbert space.
**S1.00089 Variational Approach to a Class of P-T Symmetric Hamiltonian Systems**, J. MIKALOPAS, J.D. MANCINI, Kingsborough College of CUNY, Brooklyn, NY, V. FESSATIDIS, Fordham University, Bronx, NY, F.A. CORVINO, Stevens Institute of Technology, Hoboken, NJ — In the usual study of non-relativistic Quantum Mechanics, one chooses a real (Hermitian) potential so as to ensure a real energy spectrum for the corresponding Schrödinger equation. In recent years, a number of authors have studied a class of complex potentials which are invariant under the combined symmetry P-T (here the operator $P$ represents parity reflection and the operator $T$ represents time reversal). For such P-T symmetric systems it has been shown that the energy eigenvalues of the Schrödinger equation are real so long as the P-T symmetry is not spontaneously broken. Thus it would appear that rather than the usual demand for Hermiticity, it may be sufficient to have a P-T invariant Hamiltonian so long as the energy spectrum remains real. It should be noted however that this conjecture has not been proven, but rather has been demonstrated to be true for several sample Hamiltonian systems. Here we wish to apply a recently developed ansatz wherein a variational basis is constructed by systematically taking derivatives of an initial trial state with respect to a (set) of variational parameters. In particular we shall study the spectrum of the Hamiltonian $H = p^2 + x^2 (ix)^a$ (a real) as a test case for the ansatz.

**S1.00090 Single Hole Dynamics in a 2D quantum antiferromagnet in a stripe-ordered by fluctuating background**, SATYAKI KAR, Department of Physics, FSU, EFSTRIATOS MANOUSAKIS, Department of Physics, FSU & MARTECH — We study the dynamics of a hole in a 2D lattice in a stripe-ordered background. Starting from $t - J$ Hamiltonian, we treat the $J$-term using the linear spin wave theory and we linearize the hole hopping in terms of spin-deviation operators. We find the dispersion relation of the eight different spin-wave modes and we solve the Dyson’s equation with the non-crossing approximation for the eight hole green’s functions. We investigate the hole energy bands, the spectral functions and the quasi-particle peak broadening.

**S1.00091 Towards a two dimensional lattice gas with dynamical geometry**, ANNA KLALES, DONATO CIANCII, ZACHARY NEEDELL, PETER LOVE, Haverford College — We report on simulations using a lattice gas automaton in which the lattice is replaced by a triangulation of an arbitrary two-dimensional manifold. If the manifold is 2D Euclidean space the particles move on the Kagome lattice. We report results of simulations of channel flow for the flat space model and of simulations in which the particle state can change the geometry of the triangulation through the Pachner moves.

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1Supported by Research Corporation and Howard Hughes Medical Institute

**S1.00092 Quantum Monte Carlo Studies of Buckling of the Si(100) Surface**, WENDY LAMPART, RICHARD CHRISTIE, DANIEL SCHOFIELD, KENNETH JORDAN, University of Pittsburgh Department of Chemistry — The quantum Monte Carlo method is used to study the role of electron correlation on the buckling of Si-Si dimers on the Si(100) surface. The buckling is addressed using cluster models with one to three surface dimers. In addition to the diffusion Monte Carlo method, calculations are also carried out using various density functional methods, multi-reference MP2, multi-reference MP3, and approximate multi-reference coupled cluster approaches. The calculations show that high-order correlation effects are important for determining the relative stability of the buckled and unbuckled structures, favoring the buckled structure.

**S1.00093 Quantum Monte Carlo study of water-acene systems**, JIAWEI XU, RICHARD CHRISTIE, KENNETH JORDAN, University of Pittsburgh — Electronic structure quantum Monte Carlo methods are used to calculate the energies of a water molecule interacting with benzene, anthracene, and coronene. Localized orbitals represented as spline functions are used to reduce the computational cost of the calculations for larger water-acene complexes. The prospects of using this approach to determine the interaction energy between water and graphene is discussed.

**S1.00094 Ab initio study of ferroelectricity in quantum-confined nanostructures**, GHANSHYAM PILANIA, RAMAMURTHY RAMPRASAD, University of Connecticut — In the present ab initio study, we have employed density functional theory to investigate the size dependence of ferroelectric properties of BTO quantum wires and quantum dots. In the case of quantum wires, the ferroelectric well depth was calculated as a function of size. We find that the ferroelectric well depth corresponding to bulk BTO is recovered in quantum wires with diameters larger than 1 nm. Analysis of the decomposed density of states indicates that the central BTO unit behaves bulk like, whereas the peripheral units result in defect states in the band gap (with density depending on facet terminations). Complex polarization patterns were also observed, and were strong functions of the surface termination of the nanostructures. For instance, in non-stochiometric quantum wires with all surface facets terminated with TiO2, strong axial polarization was dominant. However, in BaO terminated quantum wires, polarization in the “shell” region is radial, while in the “core” region the polarization is axial. The BTO quantum dots that were studied displayed even more complex polarization patterns, reminiscent of the “vortex” patterns anticipated earlier based on effective hamiltonian calculations.

**S1.00095 On the interplay between spin polarization, orbital polarization and spin-orbit coupling in actinides from Pa to Cm**, MD ISLAM, ASOK RAY, University of Texas at Arlington, TX 76019 — We present a systematic investigation of the effects of spin polarization, orbital polarization and spin-orbit coupling in six actinide elements, namely Pa, U, Np, Pu, Am and Cm using relativistic full-potential augmented plane wave with local orbital basis method. Our calculation shows that the 5f electrons in lighter actinides are itinerant with no magnetic effects. In heavier actinides, the 5f electrons are strongly correlated and quite sensitive to spin polarization, although the difference between FM and AFM energies tends to be very small. The orbital polarization has strongest effect in NM order and nearly vanishes for spin polarized calculations in almost all cases. The 5f-electrons in α-Pu are close to being delocalized and their behavior is similar to that of lighter actinides. Among all the elements studied in this work, δ-Pu exhibits the most complex behavior. All forms of correlation effects are comparable in δ-Pu and significantly affect volume, bulk modulus and ground state energy.

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**S1.00096 Strain-dependence of the superconducting critical temperature Tc in Al and Nb simple crystals from first-principles**, M. SALVETTI, N. BONINI, M.I.T., M. CALANDRA, IMPMC/CNRS, D. PARKS, N. MARZARI, J. MIKALOPAS, M.I.T. — In the past 20 years, efforts have been devoted to predict the critical current density $J_c$ of superconducting magnets based on the Nb$_5$Sn compound. The use of Nb$_5$Sn magnets for high-field applications has highlighted the dependence of $J_c$ on strain. We present calculations of the $T_c$-dependence of Al and Nb crystals on pressure, uniaxial and shear strains using the DFT $PWscf$ package from the Quantum-ESPRESSO distribution to evaluate the phonon linewidth and the $el$-$ph$ coupling parameter using very dense k-space samplings of the IBZ. The superconducting critical $T_c$ is calculated by using the McMillan formula as a fit to the solution of the Migdal-Eliashberg equations. Favourable comparisons with available experimental data have been obtained and will be presented. The modelling of the $T_c$-dependence on strain in Nb$_5$Sn crystals is an ongoing effort. The potential for modelling the $T_c$-dependence on strain in Nb$_5$Sn is discussed. In this regard, recent advances in the implementation of the Wannier formalism give access to the sampling of the dense k-point grids required to calculate fully-converged electron-phonon coupling quantities. This approach opens the possibility to extend the study of the $T_c$-dependence on strain to unit cells characterized by a higher number of atoms or electronic complexity.
These early experiments contrast with modern tokamaks, which are comparatively quiescent and usually have relatively higher toroidal $B$ and lower $V$.

The conflict of DFT Kohn-Sham equations with the Ritz variational principle will be demonstrated rigorously. It will be shown that the ground-state charge density of the material is not representable by auxiliary one-electron orbitals of variational character. This inconsistency is also expressed by a charge-sloshing effect in attempt to solve these equations consistently.


Supported by NERSC Arkansas-Oklahoma.

S1.0099 Loop voltage, inductance, and impurity ion velocity in toroidal discharges, D. H. MCNEILL, Consultant, 3955 Bigelow Blvd., Pittsburgh, PA 15213 — Strong co-current drift and substantial heating of impurity ions were reported in some early (∼1960) toroidal devices with low magnetic field $B$ and high loop voltage. $V_L$ (Sceptre and ZETA in Britain and Alfa in Russia). High frequency spikes in $V_L$ suggest rapid changes in the discharge inductance; $V_L$ should be treated as the sum of resistive [IR] and inductive [d(LI)/dt] terms. Experimental data can be used to estimate the resistive and inductive contributions. High-energy electrons and (impurity and hydrogenic) ions were observed, but the average energies were a few tens of eV. Calculations using a 1-D momentum equation with a toroidal electric field as driver and slowing in Coulomb collisions and inelastic processes yield impurity ion (average) drift velocities and apparent temperature (drift driven by voltage spikes) that are consistent with spectroscopic observations on Alfa. These early experiments contrast with modern tokamaks, which are comparatively quiescent and usually have relatively higher toroidal $B$ and lower $V_L$. On the other hand, ZETA was a precursor of the reversed field pinch (RFP), some of whose characteristics seem related to their high $V_L$. Toroidal drift (“rotation”) velocities for tokamaks and RFPs can be calculated in the same way.

S1.00100 Finite Difference Time Evolution of the Quantum Wigner Function in the Presence of a Magnetic Field, TIMOTHY BERGSTRESSER, TOMAS MATERDEY, University of Massachusetts Boston — Numerical results from the finite-difference solution of a quantum Vlasov equation that governs the dynamics of the Wigner function in the presence of a magnetic field will be presented. Effects of absorbing boundary conditions in phase space and use of higher order finite-difference approximations will be discussed.

S1.00101 Red Shifts and Existing Speculations, SOL AISENBERG, IT GROUP — There are many current flaws, mysteries, and errors in the standard model of the universe - all based upon speculative interpretation of many excellent and verified observations. The most serious cause of some errors is the speculation about the meaning of the redshifts observed in the 1930s by Hubble. He ascribed the redshifts as due to “an apparent Doppler effect”. This led to speculation that the remote stars were receding, and the universe was expanding — although without observational proof of the actual receding velocity of the stars. The age of the universe, based upon the Hubble constant is pure speculation because of lack of velocity demonstration. The belief in expansion, the big bang, and of inflation should be reexamined. Also, the redshift cannot always be used as a distance measure, particularly for photons from quasars containing massive black holes that can reduce photon energy through gravitational attraction. If the linear Hubble constant is extrapolated to the most remote super novae and beyond, it would eventually require that the corresponding photon energy go to zero or become negative — according to Hubble linear relationship. This should give a reexamination of the meaning of the red shift and the speculative consequences and give a model with fewer mysteries.

S1.00102 Challenging the fundamental interactions in nature: Can 1/r-interactions, like the gravitational and Coulomb interactions, be induced interactions?, BO E. SERNELIUS, Linköping University — Two of the fundamental interactions in nature, the Coulomb interaction and the gravitational interaction, vary with distance as 1/r. Here we address the question if an induced, as opposed to fundamental, interaction could have this distance dependence. We show that in theory it is possible to obtain a Casimir interaction potential that varies with distance as 1/r. We achieve this by invoking hypothetical particles having a harmonic oscillator interaction potential. These particles generate fields that are different from the ordinary electromagnetic fields. The derivation parallels the derivation of the Casimir-Polder interaction between atoms in electromagnetism. The derivation relies on the harmonic oscillator interaction between the particles and Einstein’s two postulates in special relativity.

S1.00103 Reinterpreting Relativity’s Negative Solutions: An Introduction to the Theory of Symmetry Physics, B. G. SZABÓ — Using basic algebra, it can be shown that Einstein’s renowned equation $E = mc^2$ is only half correct. Just as the equation $x^2 = 9$ has two equally valid solutions, i.e. $x = +3$ and $x = -3$, there are two equally valid solutions to the useful relativistic equation: $E^2 = (pc)^2 + (mc^2)^2$. When the object is at rest ($p = 0$) $E^2 = (mc^2)^2$ or, as above $E = + mc^2$ and $E = - mc^2$. Furthermore, it can be shown that this negative solution is found throughout relativity. In general, there are two equally valid mathematical solutions to the Pythagorean theorem and this concept can be extended to the foundation of relativity – the Einstein hypotenuse. Are the negative solutions merely a mathematical curiosity or a fundamental physical reality? Current physics, discards the negative solution as not physically realizable. It is believed that this mathematically deficient practice results in physically inconsistent phenomena, e.g. the apparent matter-antimatter asymmetry, apparent CP violation, etc. However, by applying the basic premise of Symmetry Physics these phenomena have natural, experimentally falsifiable explanations: For all matter there exists equal but opposite antiamatter. Or more precisely with deference to particle/wave duality: For every particle/wave there exists an equal but opposite antiparticle/antimode. Further information can be found at http://www.symmetryphysics.com

S1.00104 Origin of Everything and the 21 Dimensions of the Universe, MARK LOEV — The Dimensions of the Universe correspond with the Dimensions of the human body. The emotion that is a positive for every dimension is Love. The negative emotion that effects each dimension is listed. All seven negative emotions effect Peace, Love and Happiness. 21st Dimension: Happiness Groin & Heart 20th Dimension: Love Groin & Heart 19th Dimension: Peace Groin & heart 18th Dimension: Imagination Wave Eyes Anger 17th Dimension: z wave / Closed Birth 16th Dimension: Electromagnetic Wave Ears Anger 15th Dimension: Universal Wave Skin Worry 14th Dimension: Lover Wave Blood Hate 13th Dimension: Disposal Wave Buttocks Fear 12th Dimension: Builder Wave Hands Hate 11th Dimension: Energy Wave Arms Fear 10th Dimension: Time Wave Brain Pessimism 9th Dimension: Gravity Wave Legs Fear 8th Dimension: Sweet Wave Pancreas Fear 7th Dimension: File Wave Left Lung Fear 6th Dimension: Breathing Wave Right Lung Fear 5th Dimension: Digestive Wave Stomach Fear 4th Dimension: Swab Wave Liver Guilt 3rd Dimension: Space Wave Face Sadness 2nd Dimension: Line Wave Mouth Revenge 1st Dimension: Dot Wave Nose Sadness The seven deadly sins correspond: Anger Hate Sadness Fear Worry Pessimism Revenge Note: Guilt is fear
S1.00106 Searching for a possible universal character of non-equilibrium fluctuations\(^1\). A. OPRISAN, College of Charleston, J. HEGSETH, University of New Orleans, S. OPRISAN, A. TEKLU, College of Charleston, C. LECOUTRE, Y. GARRABOS, D. BEYSENS, University of Bordeaux — Light scattering due to microscopic fluctuations was used to investigate possible universal laws. We used two significantly different physical systems: a pure fluid near critical temperature in microgravity and silica or gold colloids under the influence of gravity. The direct visualization and analysis of thermal fluctuations and phase separating in pure fluids near critical temperature in microgravity provides invaluable information about cooperative phenomena and the role played by the thermodynamic fluctuations in determining the critical behavior. Scattering from a non-equilibrium macroscopic concentration gradient in a free diffusion experiment for two colloidal samples under the influence of gravity is determined both by diffusion and the buoyancy. Using image processing techniques for series of recorded images from both experiments, we extracted both the static and dynamic structure factor. We implemented algorithms and extracting quantitative features from snapshots of images recorded near critical point. Additionally, the radial average of the power spectra for images recorded in both experiments presented the characteristic “ring” that determined the most likely wave number associated with the fluctuations.

\(^1\)Research supported by NASA-SCSGC grant and R&D grants from the CoC to A. Oprisan and S. Oprisan, NASA grants NAG3-1906 and NAG3-2447 to J. Hegseth.

S1.00107 Electronic Structure of Aluminum compounds\(^1\). A.R. CHOURASIA, Dept. of Physics, Texas A&M University-Commerce, HONG DONG, S.D. DESHPANDE, Aurangabad University, India — The valence and conduction bands of aluminum and aluminum compounds (AlB, AlN, and AlO\(_2\)) have been studied using a DFT computational approach implemented in CRYSTAL06. The Becke exchange with the LYP correlation has been employed. The atomic basis sets with diffuse and polarization functions have been optimized for each configuration in these materials. The density of states in the valence and conduction bands has been computed in each case. The projected density of states of the constituents has also been computed. The correlation between the partial density of states and the chemical bonding will be presented.

\(^1\)Work supported by Research Corporation and Organized Research, TAMU-Commerce.

S1.00108 Insights into the structure of the stable and meta-stable (GeTe)\(_m\)(Sb\(_2\)Te\(_3\))\(_n\) compounds\(,\) JUAREZ L.F. DA SILVA, ARON WALSH, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA, HOSUN LEE, Dept. of Applied Physics, Kyung Hee University, Suwon 446-701, South Korea — Phase-change materials such as (GeTe)\(_m\)(Sb\(_2\)Te\(_3\))\(_n\) (GST) have been considered as one of the most natural candidates for the development of non-volatile memory devices, however, there is no common consensus on the structure of these compounds. Using first-principles calculations, we identify the mechanisms that lead to the lowest energy structures for the crystalline GST compounds, namely, strain energy release by the formation of superlattice structures along the direction and by maximizing the number of Te atoms surrounded by three Ge and three Sb atoms (3Ge-Te-3Sb rule), and Peierls-type bond dimerization. The intrinsic vacancies form ordered planes perpendicular to the stacking direction in both phases, which separate the GST building blocks. The 3Ge-Te-3Sb rule leads to the intermixing of Ge and Sb atoms in the (001) planes for Ge\(_3\)Sb\(_2\)Te\(_6\) and Ge\(_3\)Sb\(_2\)Te\(_7\), while only single atomic species in the (001) planes satisfy this rule for the Ge\(_3\)Sb\(_2\)Te\(_7\) and Ge\(_3\)Sb\(_2\)Te\(_8\) compositions.

S1.00109 TEM study of Pt nanoparticles on gamma Al\(_2\)O\(_3\)/NiAl support\(\)\(\). ZHONGFAN ZHANG, LONG LI, JUDITH YANG, UNIVERSITY OF PITTSBURGH TEAM — Pt gamma Al\(_2\)O\(_3\) as one of the most important catalysts has attracted much attention in research. Moving beyond the current phenomenological understanding of the nanoparticle support interaction necessitates the examination of the Pt/\gamma-Al\(_2\)O\(_3\) interface at the atomic level. To produce the model interface, NIAF(110) single crystal was oxidized at 1223K in order to fabricate gamma Al\(_2\)O\(_3\)(440). The crystallinity and uniformity of the oxide film was characterized by X-ray diffraction (XRD). Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). Nanometer sized Pt particles were deposited through vapor deposition method onto the film. Cross-sectional TEM samples were prepared using a Focused Ion Beam (FIB). The Pt gamma Al\(_2\)O\(_3\) interface will be examined by cross-sectional transmission electron microscopy (TEM) methods to elucidate the atomic, defect and electronic structure of the interface.

S1.00110 Structural properties and electronic structures of amorphous HfO\(_2\)/Si(001) interface\(\). CHEN GUOHONG, HOU ZHUFENG, GONG XINGAIO, Surface Physics Laboratory and Department of Physics, Shanghai-200043, XGGONG’S GROUP TEAM — Using the projector augmented wave method within the generalized gradient approximation, we have performed \textit{ab-initio} molecular dynamics simulations to generate an atomic structure model of amorphous hafnium dioxide (\(\alpha\)-HfO\(_2\)) by a melt-and-quench scheme, and have investigated the structural and electronic properties of \(\alpha\)-HfO\(_2\) interface. The structure of \(\alpha\)-HfO\(_2\) sample is analyzed via atomic coordination number and partial pair-radius distribution functions. Our results show the average Hf-O nearest-neighbor distance is 2.06  \(\AA\), which is comparable with the Hf-O bond lengths (in the range from 2.04 \(\sim\) to 2.25 \(\sim\)) in monoclinic HfO\(_2\) crystalline, and also indicate the generated sample essentially reflects the experimentally measured structural characteristics of \(\alpha\)-HfO\(_2\). Most importantly, it is found that the valence band offset of \(\alpha\)-HfO\(_2\)/Si interface is about 2.97 eV, and our results suggest that the coordination of Si atoms at interface would significantly affect the electronic properties of interface.

S1.00111 Experimental Studies of the Giant Dielectric Constant Materials CaCu\(_3\)Ti\(_4\)O\(_{12}\). JIANJUN LIU, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Nebraska, 68182-0266, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION — We present results of four different experimental studies, namely (1) scanning electron microscopy, (2) dielectric measurements, (3) \textit{in-situ} high-pressure and X-ray and (4) low-temperature specific heat, on the insulating giant dielectric constant material CaCu\(_3\)Ti\(_4\)O\(_{12}\). From analyzing the results, we first deduce the electronic and mechanical properties of the samples and conclude that the mechanism for high-dielectric constant phenomena is mostly extrinsic. In addition we propose a phenomenological model to explain the high dielectric constant behaviors at both low and high frequencies.

S1.00112 Dielectric tensors of high-\(k\) \textit{Pbnm} perovskites from first principles. SINISA COH, DAVID VANDERBILT, Rutgers University — Among the materials under consideration for future high-k dielectrics in MOSFET and other microelectronic devices are several perovskites having space group \textit{Pbnm}. Among these are LaLuO\(_3\), SrB\(_2\)O\(_3\) (B = Zr, Hf), AsCO\(_3\) (A = La, Pr, Nd, Sm, Gd, Tb, Dy), and LaB\(_2\)Z\(_2\)O\(_3\) (B = Ca, Mg) (with lower symmetry), which are all compatible with growth on silicon and can have higher dielectric constants than HfO\(_2\). Using first-principles DFT methods with ultrasoft pseudopotentials and GGA energy functionals, we compute the dielectric tensors, structural properties, and phonon spectra of these materials. We analyze the dependence of these properties on chemical composition, and compare with experiments where possible. We also focus on correlation between dielectric tensor anisotropy and octahedra rotation angles.


S1.00113 Thickness dependent multiferroicity in relaxor Pb(Fe$_{2/3}$W$_{1/3}$)O$_3$ thin films, ASHOK KUMAR, RAM S. KATIYAR, University of Puerto Rico — Epitaxial multiferroic Pb(Fe$_{2/3}$W$_{1/3}$)O$_3$ thin films were fabricated on MgO substrates by pulse laser deposition. The surface morphology indicates homogeneous distribution of grain with an average surface roughness $\sim 2.5$ nm. Highly frequency dispersive spectra were observed between 120 K to 220 K suggests relaxor-like nature of epitaxial PFW thin films. Relaxor behavior was suppressed and dielectric dispersion increased with decrease in thickness from 300 nm to 50 nm. Modified Curie-Weiss law was used to analyze the relaxor character of films. Dielectric characteristic were further studied using different DC bias field $\sim 5$ kV/cm over wide range of temperature to investigate the polarization properties below freezing temperature. The impedance spectroscopy was carried out to check the grain and grain boundary effects near the dielectric dispersion regions. Magnetization vs. applied magnetic field displayed weak ferromagnetic properties. Temperature dependent polarized Raman spectroscopy were carried out to investigate the change in crystal structure, lower frequency $F_{2g}$ phonon mode, $A_{1g}$ phonon mode near the dielectric dispersion region. In plane compressive strain plays vital role to suppress relaxor behavior in thin films compare to single crystal/bulk counterpart.

S1.00114 Multiferroic properties of artificially designed Perovskite-Spinel Heterostructures, SANDRA DUSSAN, MANOJ K. SINGH, RAM S. KATIYAR, University of Puerto Rico — Multiferroics materials are a class of functional material that combines two or more ordered parameters i.e. ferromagnetic, ferroelectric and ferroelastic. The recent finding of multiferroic composite material with the coexistence of these properties has attracted the attention of various researchers due to its potential applications in highly sensitive sensors and actuators as well as multistate memory devices. We synthesized and characterized CoFe$_2$O$_4$-BFeO$_3$ (CFO-BFO) heterostructure thin films grown on SrTiO$_3$ (111), (100) substrates using Pulsed laser deposition. The XRD patterns of CFO-BFO multilayered films evidenced that all picks correspond to CFO and BFO structure also confirmed by their respective Raman spectra. We observed three peaks at 136, 168, and 215 cm$^{-1}$ that can be assigned to $A_1$(TO) modes of the BFO pure phase and at 468 and 695 cm$^{-1}$ correspond to CFO. Room temperature M-H exhibited well-shaped magnetization hysteresis loops, good saturation and high coercivity. Preliminary results evidenced the existence of ferroelectricity and magnetic properties in heterostructure.

S1.00115 Single Phase multiferroics Pb$_x$(Zr$_{1/2}$Ti$_{1/2}$)$_{1-x}$(Fe$_{1/2}$Ta$_{1/2}$)$_x$O$_3$ thin films, DILSOM A. SANCHEZ, ASHOK KUMAR, RAM S. KATIYAR, University of Puerto Rico — The epitaxial Pb$_x$(Zr$_{1/2}$Ti$_{1/2}$)$_{1-x}$(Fe$_{1/2}$Ta$_{1/2}$)$_x$O$_3$ (PZTFT) ($x = 0.1$, 0.2, 0.3) thin films were fabricated by pulsed laser deposition. X-ray diffraction (XRD) patterns of all compositions showed single phase at room temperature without any pyrochlore phase. These materials showed good ferroelectric and ferromagnetic properties at room temperature. Room temperature multiferroicity were observed in PZTFT for $x > 10$%. PZTFT illustrated high dielectric constant and low loss at room temperature. The dielectric maximum temperature shifted to lower temperature side with increase in iron and tantalum concentration. Magnetization vs. applied magnetic field (M-H) curves showed well defined hysteresis with remanent magnetization ($\sim 0.004-0.13$ emu/gm) and very small coercive field (900 Oe). Preliminary data indicate that PZTFT is a promising candidate of room temperature multiferroic materials. AC and DC conductivity of PZTFT showed very low conductivity $\sim 10^{-9}$ to $10^{-7}$ S/cm$^{-1}$ at room temperature.

S1.00116 Abstract withdrawn —

S1.00117 Strain induced electric field driven relaxor ferroelectricity in BaZr$_{1-x}$Ti$_x$O$_3$ system, TAMNOY MAITI, Lawrence Berkeley National Laboratory, RUYAN GUO, AMAR BHALLA, The University of Texas at San Antonio — A revised complete phase diagram of Ba(Zr$_{1-x}$Ti$_x$)$_3$O$_9$ (0.0 < x < 1.0) has been developed based on evaluation of their crystallographic, dielectric, and ferroelectric properties. A new understanding of the relaxor behavior in this system, e.g. associated with the local elastic strains at the nanoscale, has been gained and presented in this paper. Two different kinds of relaxor behaviors are observed in the BZT system; one is dominated by polar Ti-rich regions and another by non-polar Zr-rich regions. BZT relaxor compositions are characterized by measurement of their dielectric (under bias), pyroelectric, and thermal expansion properties in a wide range of temperatures. The structure of the BZT compositions was evaluated by X-ray and neutron diffraction studies. Their local structure has been also probed by micro-Raman spectra. Although the global symmetry of BZT relaxors is cubic from neutron diffraction studies, non-cubic local symmetry is evident based on the micro-Raman spectra of BZT relaxors.

S1.00118 Comparative study of electronic structures and nonproportionality of scintillator materials$^1$, WAWHY SETYAWAN, Duke University, ROMANCE GAUME, ROBERT FEIGELSON, Stanford University, STEFANO CURTAROLO, Duke University — The electronic structures of selected scintillator materials for gamma-ray detection are calculated. We use Vienna Ab-initio Simulation Package with projector augmented waves pseudopotentials and exchange-correlation functionals as parameterized by Perdew-Burke-Ernzerhof. Curvatures of the top of valence band and the bottom of conduction band are calculated. Parameters are introduced to measure the degree of nonproportionality of photon response of the scintillator. The data show an interesting correlation between the band curvatures and the nonlinearity. The results can be used to guide the design of future proportional scintillators.

$^1$This research is sponsored by NSF and DHS.

S1.00119 Synthesis and Characterization of Alumina/Titania Nanofibers, R.K. FEAKER, D.A. PERHAY, John Carroll University, A.F. LOTUS, E.T. BENDER, G.G. CHASE, R.D. RAMSIER, The University of Akron, N. STOJILIVOIC, John Carroll University — Both alumina and titania nanofibers are promising materials for use in high-temperature applications. In an attempt to access the properties of these two materials systems simultaneously we synthesize alumina/titania nanofibers by electrospinning. We characterize their properties using different analytical methods (scanning electron microscopy, thermogravimetric analysis, X-ray diffraction, and infrared, and X-ray photoelectron spectroscopies). We compare the properties of these mixed fibers with pure alumina and pure titania nanofibers and investigate the effects of annealing.

S1.00120 Controlled TiO$_2$ nanoparticles on solid substrate for high gate dielectric of a pentacene based organic thin film transistor (OTFT), HIMADRI ACHARYA, JINWOO SUNG, GEUN TAK LEE, TAE HEE KIM, Department of Materials Science and Engineering, Yonsei University, Seoul 120749, Korea, BYUNG GIL KIM, School of Advanced Materials and System Engineering, Kunsan Institute of Technology, Kumi 730701, Korea, CHEOLMIN PARK, Department of Materials Science and Engineering, Yonsei University, Seoul 120749, Korea — Ordered high $\phi$ TiO$_2$ nanoparticles on substrate in large area have been developed using self assembled poly(styrene)-block-poly(4-vinylpyridine) (PS-b-P4VP) and Ti-precursors by simple spin coating method. Calcination at 600$^\circ$C in ambient atmosphere removes both blocks of the polymers from the substrate and results in well ordered arrays of TiO$_2$ nanoparticles. Subsequent spin coating of polystyrene (PS) insulator was performed to generate gate dielectric film with higher permittivity on which pentacene based organic thin film transistor (OTFT) was developed to investigate the permittivity effect on transistor performance. The arrays of TiO$_2$ nanoparticles firmly adhering to substrate exhibit a significant dielectric constant enhancement when used for capacitance measurement. The incorporation of single walled carbon nanotube (SWNT) during the formation of TiO$_2$ nanoparticles on substrate further improves the transistor behavior by electrostatic coupling of high $k$ TiO$_2$ dielectric ($\sim 80$) with SWNT.

S1.00121 SEMICONDUCTORS —
S1.00122 Low-bias Transport Features in a Quantum Point Contact with a Variable Aspect Ratio1, BRYAN HEMINGWAY, TAI-MIN LIU, ANDREI KOGAN, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University, UNIVERSITY OF CINCINNATI TEAM, XAVIER UNIVERSITY COLLABORATION, PURDUE UNIVERSITY COLLABORATION — Quantum Point Contact (QPC) devices frequently display a zero-bias conductance anomaly (ZBA), the origin of which is not fully understood. To investigate a possible connection between the ZBA and the device geometry, we use a four-gate QPC device patterned on a GaAs/AlGaAs semiconductor heterostructure, aiming to achieve independent control over the transverse and the longitudinal potential profiles. In several regimes, we find a narrow ZBA that shows a pronounced temperature dependence for T ~ 100 mK. Coulomb peaks arise under certain device settings, suggesting a weakly bound state located in the QPC. For other settings, we observe a plateau below the first conductance step. The plateau's conductance varies as the aspect ratio of the confining potential is changed. We describe a series of magnetic field measurements that show splitting of the ZBA and compare the findings to our measurements in a different, very short device which displayed no ZBA.  

1The research is supported by NSF DMR award No. 0804199 and by University of Cincinnati.

S1.00123 Magnetooptical and magnetic studies of Co and Cr doped CdMnTe, S. SHEN, X. LIU, Y.J. CHO, J. FURDYNA, M. DOBROWOLSKA, University of Notre Dame, Y.H. HWANG, Y.H. UM, University of Ulsan — We investigate the magnetooptical and magnetic properties of two new CdMnTe-based diluted magnetic semiconductors. The first system consists of a series of Cd$_{1-x-y}$Mn$_x$Co$_y$Te alloys with Mn concentration $x$ fixed at ~0.37 and controlled Cr concentration $y$ in the range $0 < y < 0.07$. The second system is the quaternary Cd$_{1-x-y}$Mn$_x$Co$_y$Te alloy, with the same Mn concentration ($x = 0.37$) and the Co concentration $y$ in the range $0 < y < 0.009$. These systems are of interest in that they are expected to involve interactions of the minority magnetic ions (Cr and Co, respectively) with the surrounding majority Mn ions. Indeed, optical absorption and MCD spectra observed on these alloys reveal a series of new “impurity” peaks that are not present in the Cd$_{0.63}$Mn$_{0.37}$Te control samples. It is interesting that the magnetic field dependence of the MCD spectra as well as SQUID measurements reveal a ferromagnetic-like hysteresis loop in Cd$_{1-x-y}$Mn$_x$Co$_y$Te samples with Cr concentration $y$ in the range of $0 < y < 0.03$. Surprisingly, the FM loop survives up to 295 K. But this ferromagnetic behavior is not observed in samples with $y > 0.05$. One should note that FM loops were not observed in Cd$_{1-x}$Mn$_x$Co$_y$Te samples.

S1.00124 Experimental investigation of spin interference phenomena in InGaAs/InAlAs rectangular loop arrays, SEBASTIEN FANIEL, TAKAAKI KOGA, GSIST and CRIS, Hokkaido University, Japan, YOSHIKI SEKINE, NTT BRL, NTT Corporation, Japan — We report spin interference experiments in rectangular loop arrays built from InGaAs quantum wells. Low $T$ magnetotransport measurements in such systems exhibit Ahuizer-Aronov-Spivak (AAS) oscillations stemming from the interference between closed loop trajectories in clockwise and counterclockwise directions. In InGaAs devices, that show a large, gate-controllable spin-orbit (SO) interaction, this interference can be tuned by means of a front gate voltage, leading to a modulation of the AAS oscillations. The present work focuses on the anisotropic interplay between the Rashba and the Dresselhaus contributions to the SO interaction. Along the [-110] and the [110] crystallographic directions, the Rashba and the Dresselhaus effective magnetic fields are expected to be added or subtracted to/from each other. To probe this anisotropy, we study rectangular loop array interferometers whose sides are aligned along these two particular crystallographic directions. We analyze our results using a model that includes both the Dresselhaus and the Rashba SO interactions and accounts for phase decoherence in the devices. This work was supported by KAKENHI (19684009) and also partially by Support Center for Advanced Telecommunications Technology Research, Foundation (SCAT).

S1.00125 Zero-field spin-splitting and spin lifetime in $n$-InSb/In$_{1-x}$Al$_x$Sb quantum wells, A.M. GILBERTSON, Imperial College, M. FEARN, J.H. JEFFERSON, QinetiQ Malvern, B.N. MURDIN, Surrey University, P.D. BUCKLE, QinetiQ Malvern, L.F. COHEN, Imperial College — The Rashba and Dresselhaus coupling parameters are calculated for a range of carrier densities in [001]-grown $d$-doped $n$-type InSb/In$_{1-x}$Al$_x$Sb quantum wells using an established 8 band k.p formalism [1]. It is shown that both sets of parameters scale approximately linearly with carrier density. In contrast to other materials the Dresselhaus contribution to spin splitting is found to be of significant and comparable value to the Rashba mechanism under certain conditions. The inherently large BIA induced SO coupling in these systems is shown to have considerable effect on the spin lifetimes for spins oriented along [110] based on D’yakonov-Perel’ mechanism [2]. The relaxation rate of spins oriented in the [001] direction is found to be dominated by the k-linear Rashba and Dresselhaus coupling parameters and at least an order of magnitude greater than in the [110] direction [3]. Comparison to recent experimental results in similar structures is presented. [1] P. Pfeffer and W. Zawadzki, PRB 59, 8 RS312 (1999) [2] Averkiev et al., J. Phys.:Condens. Matter 14 (2002) [3] A.M.Gilbertson et al., PRB 77 (16), 165335 (2008)  

1Research supported by UK EPSRC

S1.00126 Nuclear Effects on Electron Spin Resonance in Gallium Arsenide1, AARON JONES, JOHN COLTON, BENJAMIN HEATON, DANIEL JENSON, MICHAEL JOHNSON, Brigham Young University — Electron spin properties in gallium arsenide (GaAs) are investigated by electron spin resonance (ESR), the signal being detected via optical Kerr rotation. Experiments in ESR have shown broadened and shifted resonance peaks due to the hyperfine nuclear interaction. Simultaneous nuclear magnetic resonance (NMR) reduces the nuclear effects by preventing the nuclei from responding to the changing electron polarization. However, low NMR power still permits the electron spins to have a great effect on the nuclei, which then affect the electrons in return. We have developed a tunable, impedance-matched, lumped-element rf circuit which increases the output power at the resonant frequency of the three nuclei $^{119}$As, $^{71}$Ga, and $^{69}$Ga. Improved ESR data resulting from stronger NMR is presented.  

1This work was supported by NSF grants 0419501, 0456074, and 0802831

S1.00127 ABSTRACT WITHDRAWN —

S1.00128 Generation of spin polarized current in a semiconductor by an ohmic contact containing ferromagnetic particles, LEONARDO CASTELANO, Department of Physics, University of California, San Diego, YU-CHANG CHEN, Department of Electrophysics, National Chiao Tung University, S.-R. ERIC YANG, Physics Department, Korea University, LU SHAM, Department of Physics, University of California, San Diego — We investigate the possibility of injection of spin polarized current into a semiconductor from an ohmic contact containing ferromagnetic metal (FM) nanodots. The polarization is created by the spin-dependent scattering of the current carriers with the FM dots with aligned magnetizations. The usually inefficient polarization generation due to the resistance mismatch between the metal electrode and the semiconductor is mitigated by the reduction of the mismatch between the FM dots and the heavily doped electrode. When the paramagnetic semiconductor is connected by two such electrodes containing FM dots forming a spin valve system, the magnetoresistance is calculated to be sizable. We report the calculation results for two examples: (i) silicon connected to electrodes of poly-silicon contain the FM dots and (ii) the heavily doped region of InAs as contact.  

1This work is supported by ARO-MURI on Magnetic Dynamics and in part by CNPq (Brazil).
S1.00129 Spin polarization of doped II-VI nanocrystals, SAVAS DELIKANLI, WILLIAM FALLS, MESUT YASAR, ATHOS PETROU, HAO ZENG, Department of Physics, University at Buffalo-SUNY — The photoluminescence of Mn2+ doped CdSe nanoparticles synthesized by solution phase method has been studied as a function of nanocrystal size and the circular polarization of the light emitted from Cd1−xMnxSe nanoparticles has been investigated as a function of an applied magnetic field in the 7-100 K temperature range. Spin polarized photoluminescence emission from Cd1−xMnxSe was observed and strongly depends on the growth time of the nanoparticles. They show negatively polarized photoluminescence emission and the behavior of spin polarization strongly depends on the applied field. Spin polarization initially saturates between 1-3 Tesla and shows an unexpected linear increase beyond 3 Tesla. Magnetization of Cd1−xMnxSe nanoparticles shows mostly paramagnetic behavior with some hysteresis at low temperatures.

S1.00130 Effect of pressure on spin-carrier interactions in Sb2−xVxTe3 and Sb2−xCrxTe3 single crystals1, MATTHEW L. BOWERS, JEFFREY S. DYCK, John Carroll Univ., CESTMIR DRASAR, PETR LOSTAK, University of Pardubice, Czech Republic — Bulk, single crystal samples of diluted magnetic semiconductors Sb-rich and N-poor Mn3−xSc1+xN and Fe0.1Sc0.9N films Grown by Molecular Beam Epitaxy, HAN-JONG CHIA, University of Texas at Austin, COSTEL CONSTANTIN, Seton Hall University, KANGKANG WANG, ABHIJIT CHINCHORE, ARTHUR SMITH, Ohio University, JOHN MARKERT, University of Texas at Austin — We report SQUID magnetic measurements on N-poor Mn3−xSc1+xN and Fe0.1Sc0.9N films grown on ScN(001)/MgO(001) substrates by radio frequency plasma assisted molecular beam epitaxy. Ferromagnetism is present in both the Mn doped (x ranging from 3 to 15%) and the Fe doped ScN samples. Measurements on N-poor Mn3−xSc1+xN and Fe0.1Sc0.9N films show Curie temperatures of 383 K and 361 K, respectively. The Fe0.1Sc0.9N film shows a Curie temperature above 350 K as well. Further studies will be required to determine the origin of the ferromagnetism and the Curie temperature of the remaining Mn3−xSc1+xN films. This work is supported by: Seton Hall: University Research Council; Ohio University: DOE-BES Grant No. DE-FG02-06ER46317 and NSF Grant No. 0730257; and UT Austin: NSF Grant Nos. DMR-0605828 and DGE-0549417, Welch Foundation Grant No. F-1191.

S1.00131 SQUID measurements of Mn3Sc(1−x)N and Fe0.1Sc0.9N Films Grown by Molecular Beam Epitaxy, HAN-JONG CHIA, University of Texas at Austin, COSTEL CONSTANTIN, Seton Hall University, KANGKANG WANG, ABHIJIT CHINCHORE, ARTHUR SMITH, Ohio University, JOHN MARKERT, University of Texas at Austin — We report SQUID magnetic measurements on N-rich and N-poor Mn3Sc(1−x)N and Fe0.1Sc0.9N films grown on ScN(001)/MgO(001) substrates by radio frequency plasma assisted molecular beam epitaxy. Ferromagnetism is present in both the Mn doped (x ranging from 3 to 15%) and the Fe doped ScN samples. Measurements on N-poor Mn3Sc(1−x)N and Fe0.1Sc0.9N films show Curie temperatures of 383 K and 361 K, respectively. The Fe0.1Sc0.9N film shows a Curie temperature above 350 K as well. Further studies will be required to determine the origin of the ferromagnetism and the Curie temperature of the remaining Mn3Sc(1−x)N films. This work is supported by: Seton Hall: University Research Council; Ohio University: DOE-BES Grant No. DE-FG02-06ER46317 and NSF Grant No. 0730257; and UT Austin: NSF Grant Nos. DMR-0605828 and DGE-0549417, Welch Foundation Grant No. F-1191.

S1.00132 Probing current and temperature effects on the direct insulator-quantum Hall transition, KUANG YAO CHEN, C.-T. LIANG, Dept Phys, NTU, N. AOKI, Y. OCHIAI, Dept Elect & Mech Engn, Chiba Univ, K.A. CHENG, Dept Elect Engn, Chung Hwa Univ Sci & Technol, LI-HUNG LIN, Grad Inst Optoelect & Solid State Elect, NCTU, C.F. HUANG, C.M.S/ITRI, YU-RU LI, YEN SHUNG TSENG, CHUN-KAI YANG, Deps Phys, NTU, PO-TSUN LIN, Grad Inst Optoelect & Solid State Elect, NCTU, JAU-YANG WU, SHENG-DI LIN, Dept Elect Engn, NCTU — We report a magneto-transport study on the two-dimensional electron system (2DES) in an AlGaAs/Gas heterostructure. The direct insulator-quantum Hall transition is observed at different temperatures by increasing the magnetic field B perpendicular to the 2DES. Such a transition can also be observed by varying the current I since the electron temperature is given by IX = CI/2 in both the insulator and quantum Hall sides of the transition. Here α denotes the exponent for the power law and C is a constant at a particular magnetic field. The value of α may be determined by comparing the temperature and current dependences. Our results show that α takes on different values on either sides of the transition point, indicating the presence of different heating mechanisms in the low-field insulator and in the quantum Hall liquid. The effects due to electron-electron interaction and scattering are also discussed.

S1.00133 The Quantum Hall Effect Revisited, TOBIAS KRAMER, University Regensburg, E.J. HELLER, R.E. PARROTT, Harvard University, C.-T. LIANG, National Taiwan University, C.F. HUANG, National Measurement Laboratory, Taiwan, K. Y. CHEN, National Taiwan University, L.-H. LIN, National Chiao Tung University, Taiwan — Experiments shown here reveal inflection points of the Hall resistivity at half-integer filling factors 5/2 and 7/2 which become more pronounced with increasing current density up to high current. These features contradict the edge-state picture of the quantum Hall effect (QHE) and also the disorder picture of the QHE, which cannot explain a gap directly in the middle of a Landau level. We present a novel approach to the quantum Hall effect, which allows us to calculate the electronic transport in a highly non-uniform Hall field, which is present in two opposite corners of a Hall bar, the hot-spots. Precisely in one corners of the hot-spots are injected into the device and we derive the local density of states there. We obtain a self-consistent equation for the current-voltage relation through the Ohmic contact and thus a computable theory of the quantum Hall effect, which predicts a unique modulation and splitting of Landau levels caused by the presence of a high electric field exactly in line with the experimental observations.

S1.00134 The doubling of von Klitzing’s constant h/e², KESHAV SHRIVASTAVA, University of Malaya — The Hall resistivity is found to become a function of spin. For positive spin, one value is obtained but for negative sign in the spin, another value occurs. In this way, there is never only one value of the resistivity but there is doubling of values. The value of the von Klitzing’s constant is a special case of more general dependence of resistivity on the spin. We investigate the case for both high and low temperatures, for extreme quantum limit, n=0, the effective charge of the electron becomes (1/2)e. The fractional charge arises for finite value of the angular momentum. The fractional as well as the integral values of the charge are in full agreement with the experimental data. The generalized constant is h/[1/2]ge or which under special conditions becomes h/e² which is the von Klitzing’s constant [1]. [1] K. N. Shrivastava, Phys. Lett. A 113,435(1986); A326,469(2004); Mod. Phys. Lett. A 13,1087(1999); 14,1009(2000); AIP Conf. Proc. 909, 43-49(2007); 909,50-56(2007);1017, 422-428(2008);1017,326-330(2008); 1017, 47-56(2008), Proc. SPIE(USA)7155,71552F-8[7155,86](2008).

S1.00135 Correlating exciton localization with compositional fluctuations in InGaAs/GaAs quantum wells grown on the GaN (0001) and (1-101) surfaces, DANIEL RICH, STANISLAV KHATSEVICH, Ben-Gurion University, XINGANG ZHANG, DANIEL DAPKUS, University of Southern California — We have used spatially and temporally resolved cathodoluminescence to study the growth of InGaN/GaN quantum wells grown on GaN (0001) and (1-101) surfaces. The effects of In migration during growth on the resulting QW thickness and composition were examined. We employed a modified variable temperature-time resolved CL imaging approach that enables a spatial correlation between regions of enhanced exciton localization, luminescence efficiency, and radiative lifetime with the aim of distinguishing between excitons localized in In-rich quantum dots and those in the surrounding Ga-rich QW regions. A thermally activated nonradiative recombination model was invoked to explain a reversal in the spatial dependence of lifetime between cases of high and low temperatures, in which we show that nonradiative recombination is linked to an enhanced exciton dissociation at high temperatures.
S1.00136 Enhanced Luminescence in an amorphous AlN:Ho thin film by co-doped Gd+3 Cathodoluminescence

MUHAMMAD MQBOOL, Ball State University, HUGH RICHARDSON, MARTIN KORDESCH, Ohio University — Sputter deposited thin films of amorphous AlN:Ho (1 at. %) emits in the green (549 nm) region of the visible spectrum under electron excitation. The addition of Gd (1 at. %) in the film enhances the green emission linearly after thermal activation at 900 °C for 40 minutes in a nitrogen atmosphere. The luminescence enhancement saturates when the gadolinium concentration reaches four times the holmium concentration. The optical bandgap of amorphous AlN is about 210 nm, so that the film is transparent in the ultraviolet, allowing us to observe the ultraviolet emission at 313 nm from Gd. No significant quenching of the Gd emission is observed. EDX spectra confirm the increasing concentration of Gd. XRD analysis shows no peaks other than those arising from the Si (111) substrate, confirming that the films are amorphous.

S1.00137 The carrier property of Al$_{2}$Ga$_{1-x}$N/GaN nanowire fabricated by a dual-beam focused ion beam$^{1}$

JENN-KAI TSAI, Department of electronic engineering, National Formosa University, Yunlin, Taiwan, Republic of China., W.Y. PANG, Y.H. CHANG, IKAI LO, Department of Physics, Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China. — In this study, the Al$_{2}$Ga$_{1-x}$N/GaN high electron mobility transistor structure was grown on GaN template substrate using a radio frequency plasma assisted molecular beam epitaxy. The undoped GaN template substrate was grown on c-sapphire substrate by metal organic vapor phase epitaxy system. The carrier property was performed by a Hall effect measurement. The mobility and carrier density obtained of the as-grown HEMT was 1814 cm$^2$/V s and 1.29x10$^{14}$ cm$^{-2}$, respectively. The nanowire was patterned on the Al$_{2}$Ga$_{1-x}$N/GaN heterostructure by a dual-beam focused ion beam. The first step was to process a Hall bar pattern. The second step was to reduce the width of active channel. The wire width of 100 nm of nanowire was fabricated successfully. The carrier property of nanowire was evaluated at the different temperature from 4 to 300 K.

$^{1}$The authors would like to acknowledge Epistar corporation for supply GaN template substrates and financial support from the National Science Council of Republic of China(NSC 97-2112-M-150-002).

S1.00138 Magneto-transport Study on the nanometer-scaled quantum-ring interferometer made of Al$_{2}$Ga$_{1-x}$N/GaN heterostructures

WEN-YUAN PANG, IKAI LO, YU-CHI HSU, YEN-LIANG CHEN, MING-HONG GAU, YUNG-HSI CHANG, YING-CHEI WANG, JIH-CHEN CHIANG, Department of physics, National Sun Yat-sen University, Kaohsiung, Taiwan, Republic of China., JEN-KAI TSAI, Department of electronic engineering, National Formosa University, Yunlin, Taiwan, Republic of China. — The quantum-ring interferometer has been proposed for spintron ic application. The Al$_{2}$Ga$_{1-x}$N/GaN samples were grown on GaN-template buffer layer by plasma-assisted molecular beam epitaxy. The mobility and carrier density of two-dimensional electron gas to be 19845 cm$^2$/Vs and 5.18x10$^{12}$ cm$^{-2}$ by conventional van der pauw Hall measurement at temperature of 4.2 K, respectively. The samples were used to fabricate quantum-ring field-effect-transistors with different widths of conducting channel by Focus Ion Beam. The magneto-resistance measurement at temperature of 0.35 K and magnetic field up to 12 T was performed on these samples. The electronic characterization of nanometer-scaled quantum-ring made of high-mobility Al$_{2}$Ga$_{1-x}$N/GaN heterostructures has been studied.

$^{1}$The project is supported by the grant number NRC 95-2112-M-110-017-MY3 and FA8669-07-1-4022.

S1.00139 High Electron Mobility Al$_{2}$Ga$_{1-x}$N/GaN Heterostructures Grown by PAMBE on GaN Templates Prepared by MOCVD

YEN-LIANG CHEN, WEN-YUAN PANG, MING-HONG GAU, YU-CHI HSU, WAN-TSANG WANG, JIH-CHEN CHIANG, IKAI LO, Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan, ROC., CHIA-HO HSIEH, Institute of Material Science and Engineering, National Sun Yat-Sen University, Kaohsiung, Taiwan., JEN-KAI TSAI, Department of Electronic Engineering, National Formosa University, Yunlin, Taiwan, ROC. — A series high mobility Al$_{2}$Ga$_{1-x}$N/GaN heterostructures samples were grown on MOCVD-grown GaN templates by molecular beam epitaxy with different Al fractions (x = 0.017−0.355). The highest mobility in this series samples at liquid nitrogen temperature is 14110 cm$^2$/Vs with carrier concentration 2.87 x 10$^{12}$ cm$^{-2}$ and Al fraction x = 0.022. In our experiments, the carrier density decreases as Al content reduces. While the carrier density decreases from 1.54 x 10$^{13}$ cm$^{-2}$ to 2.87 x 10$^{12}$ cm$^{-2}$, the mobility increases. But as the carrier density decreases from 2.87 x 10$^{12}$ cm$^{-2}$, the mobility decreases.

$^{1}$The project is supported by National Research Council of Taiwan (NRC 95-2112-M-110-017-MY3) and by AFOSR/AOARD (AFMC, USAF) under grant number FA8669-07-1-4022.

S1.00140 Electron heating in disordered 2DEG GaAs/AlGaAs structures by THz radiation

RAHUL RAMASWAMY, YAI WANG, MATTHEW BELL, ANDREI SERGEEV, ALEKSANDR VEREVKIN, GOTTFRIED STRASSER, VLADIMIR MITIN, University at Buffalo, DAROLD WOBSCHALL, Ensensors Inc. — While numerous applications of heterostructures with two-dimensional electron gas (2DEG) in electronics require high-mobility of carriers, slow momentum relaxation creates substantial problems for employing these structures as various detectors of electromagnetic radiation. Significant kinetic inductance of carriers does not allow one to use 2DEG-based sensors in combination with ordinary antennas and readouts, designed for Ohmic detectors. Keeping in mind sensor applications, we investigate the electron heating in disordered AlGaAs/GaAs structures at liquid nitrogen temperatures. In our experiments, 2DEG was overheated by DC current or THz radiation. The devices were fabricated from AlGaAs/GaAs structures and have widths of 50-150 µm and lengths varying from 3-50 µm. 2DEGs of various levels of disorder are used to change the kinetic inductance of our devices and to study effects of disorder on electron heating. Steady-state and quasi-optical THz heating measurements provide consistent data and allows us to determine basic parameters, such as electron-phonon relaxation rate, electron heat capacity of 2DEG, and radiation coupling.

$^{1}$This research was supported by NYSTAR and NSF SBIR

S1.00141 High-Frequency Electron Pumps used as an Entangler

S. J. WRIGHT, Cavendish Lab, Cambridge, GODFREY GUMBS, Hunter College/CUNY, MICHAEL PEPPER, M. D. BLUMENTHAL, Cavendish Lab, Cambridge, DANHONG HUANG, USAF Research Lab — We calculate the exchange interaction of two interacting electrons that are captured in the quantum dot (QD) formed by the DC electric potential applied to a pair of gates. A gigahertz AC pulse is applied to one of the gates to pump electrons from below the Fermi level. We shall discuss the mechanism for capturing and ejecting electrons from the quantum dot and the characteristics of the pumped current as a function of the DC voltage. A simple model for the observed temperature dependence of the pumped current will be presented. The measured current shows plateaus at $Nf$, where $N = 1, 2, \cdots, e$ is the magnitude of the electron charge and $f$ is the frequency of the pulse. The QD capturing the electrons is modeled by a harmonic confining potential. We calculate the spin singlet and spin triplet energies which then determine the exchange interaction for $N = 2$. As the QD moves from just above the Fermi level to a height when the electrons are ejected, the confinement is strong just after the capture but the size of the QD continues to increase. When the size of the QD is increased, we show that the energy of the spin singlet and spin triplet state gets larger over a range of values for the size of the QD. We will present calculated results for the energies of entangled electrons and possible related experiments.

$^{1}$Supported by contract FA 9535-07-C-0207 of AFRL.
S1.00142 TEM analysis of Microstructure of AlN/sapphire grown by MOCVD1. B. CAI, M. L. NAKARMI, Department of Physics, Brooklyn College of the City University of New York — AlN and Al-rich AlGaN have emerged as promising deep ultraviolet (UV) materials for the development of deep ultraviolet optoelectronic devices such as light emitting devices and detectors in the spectral range down to 200 nm. High quality AlN/sapphire can be used as templates to grow nitride based ultraviolet and deep ultraviolet photonic devices due to high thermal conductivity and transparency of the light. The performance of the devices depends on the microstructures of the templates. We report on the microstructure analysis of AlN epilayer grown on sapphire. Both plane and cross section views are investigated by high resolution transmission electron microscopy. It has been revealed that the dislocations are greatly reduced by using high temperature buffers. Density of edge dislocations dominates the total density of dislocations. The microanalysis of Al-rich AlGaN epilayers grown on AlN/sapphire templates will also be presented. Implications of our finding for the applications in deep UV optoelectronic devices will be discussed.

1supported by PSC-CUNY

S1.00143 Reduction of the Specific Contact Resistance in p-type GaN-based Devices via Polarization Doping1. JACOB MELBY, JASON GU, LI HUANG, Carnegie Mellon, YUHREN WU, LISA PORTER, ROBERT DAVIS, Carnegie Mellon — The power efficiency of GaN-based devices is sensitive to energy loss at p-type semiconductor contacts. Low resistance contacts to p-type GaN are difficult to achieve due to limitations in extrinsic acceptor doping. These limitations can be avoided via polarization doping. Au/Ni contacts deposited on a 2nm thick strained In$_x$Ga$_{1-x}$N capping layer atop a p-type GaN layer exhibited three orders of magnitude reduction in the specific contact resistance versus the single layer p-type GaN control. Increased band bending near the interface due to the polar field resulted in a reduced tunneling barrier width and a decrease in the specific contact resistance. At a minimum critical capping layer thickness, a two-dimensional hole gas (2DHG) forms in the In$_x$Ga$_{1-x}$N layer. The effect of the composition and thickness of the capping layer on the specific contact resistance and the hole concentration in a 2DHG has been determined.

S1.00144 Kinetic Monte Carlo Simulation Studies of Nanocolumn Formation in Two-Component Epitaxial Growth2. SHU ZHENG, University of Tennessee & Oak Ridge National Laboratory & Dalian University of Technology, China, WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, G. MALCOLM STOCKS, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee — Recent experimental studies have revealed that well-ordered one-dimensional column structures are formed via self-assembly during two-component epitaxial growth of a variety of materials, including diluted magnetic semiconductors and high-Tc superconductors. Here we use kinetic Monte Carlo simulations to study the morphological evolution of a two-component epitaxial system, based on a (1+1)-dimensional lattice model. We find that in systems where the atom-atom interactions obey the relationship of $E_{AA} + E_{BB} - 2E_{AB} < 0$, ordered nanoscale columns can be formed during the growth. The dependence of the ordering on the growth temperature and deposition rate and on the relative concentration of the two components is also explored.

2Department of Energy

S1.00145 ABSTRACT WITHDRAWN —

S1.00146 Improved conductivity observed in doped layered oxysulfides [Cu$_2$S$_2$][Sr$_{n+1}$M$_n$O$_{3n-1}$]1. KOICHI USHIYAMA, The University of Tokyo, HIRAKU OGINO, SHIGERU HORII, JUN-ICHI SHIMOYAMA, KOHJI KISHIO — [Cu$_2$S$_2$][Sr$_{n+1}$M$_n$O$_{3n-1}$] is a group of semiconductor oxysulfides which are composed of alternate stackings of Cu$_2$S$_2$ antifluorite layers and perovskite-based M$_2$O$_3$ planes1. Perovskite structures are expected to show interesting properties such as high-temperature superconductivity and magnetoresistance. However they have attracted less attention because they have relatively high resistivity and there are only a few reports of carrier doping2. In this study, we found Na substitution was especially effective on [Cu$_2$S$_2$][Sr$_2$CoO$_2$]. Systematic decreases in lattice parameter with increasing doping levels indicated that Na was successfully substituted at the Sr site. Remarkable decrease in resistivity was observed especially at low temperatures, from 10$^3$ Ωcm (undoped) to 0.15 Ωcm at 50 K. This value is lowest ever reported in the [Cu$_2$S$_2$][Sr$_{n+1}$M$_n$O$_{3n-1}$] oxysulfides. [1] K. Ueda et al., Chem. Mater. 13 (2001) 1880 [2] K. Ito et al., J. Appl. Phys. 99 (2006) 08F705

S1.00147 Temperature dependent structural disintegration of delafossite CuFeO$_2$. P. SHOJAN, ASHOK KUMAR, RAM KATIYAR, University of Puerto Rico — Single phase delafossite p-type CuFeO$_2$ (CFO) semiconductor was synthesized by modified solid state reaction technique. X-ray diffraction (XRD) and X-ray photo spectroscopy (XPS) studies suggest pure phase of CFO and Energy dispersive X-ray spectroscopy (EDX) also revealed that the atomic ratio Cu and Fe is 1:1. The XPS spectra showed two intense Cu 2p3/2 and 2p1/2 peaks at 932.5 eV and 952 eV and two Fe 2p3/2 and 2p1/2 peaks at 710 eV and 725 eV suggesting Cu and Fe ions are in +1 and +3 state with high spin S=5/2. The room temperature Raman spectra of CFO displayed two main strong active modes at 351 cm$^{-1}$ and 692 cm$^{-1}$ that matched with other delafossite structure. Temperature dependent Raman spectra indicate that the lowest mode vanished or overdamped at ~ 400 K where as higher modes shifted to lower frequency side with significantly decreased in intensity. We have also observed a low frequency (E$_2$(low)) mode at 79 cm$^{-1}$ using 532 nm (~5MHz line width) laser line. The line width and intensity of the lowest mode indicates temperature independent behavior. Raman Spectra were carried out from 80 K to 1300 K which revealed structural disintegration in CFO over 800 K in air. The structural degradation is counter confirmed by XPS, XRD, DTA measurements. Around 800 K in air, CFO disintegrates to form CuO and CuFe$_2$O$_4$.

S1.00148 Structural and transport studies on nanostructured SnS synthesized by solvothermal process , PRATIMA AGARWAL, Department of Physics, IIT Guwahati, Guwahati 781039, India. GOURI S. PAUL, Center for Energy, IIT Guwahati, Gwahati 781039, India — Nanostructured SnS has a lot of interest due to its potential application in optoelectronic devices such as solar absorber, near-infrared detector and as a holographic recording medium. SnS usually exhibits p-type conduction and reported to have a direct band gap of about 1.32-1.5 eV and an indirect band gap of 1.1-1.3 eV dependent of the condition of preparation. In this work we report structural and transport studies on nanostructured SnS synthesized by solvothermal process for different reaction time (RT). Structural and morphological analyses are carried out by XRD, SEM and TEM. It is observed that structure of the as-prepared SnS powder samples vary with RT. SAED patterns reveal that as synthesized SnS are single crystals. Transport measurements done on thin films prepared by Doctor’s blade techniques show that films are thermally stable and uniform through out the surface. The conductivity of the SnS thin films is measured in coplanar geometry in the temperature rang (303–463) K. The films show thermally activated conduction and the curves are identical for both heating and cooling cycle.
S1.00149 Weak ferromagnetism in single crystalline Zn$_1-x$Co$_x$O thin films . H.-J. LEE, B.-G. PARK, Department of Physics, POSTECH, J.-Y. KIM, Pohang Accelerator Laboratory, POSTECH, J.-H. PARK, Y. H. JEONG, Department of Physics, POSTECH — Diluted Magnetic Semiconductors (DMS) have been actively searched for many years; a prospect of spintronic devices. Transition metal doped oxide materials, especially ZnO-based DMS, have been of particular interest as a high Tc material. Co doped ZnO thin films, for example, were reported to show ferromagnetic properties at room temperature. However, various subsequent studies including ours do not seem to converge on a definite picture and controversy continues. The observed ferromagnetism in DMS is very sensitive to the preparation methods and conditions. Therefore, what is needed to resolve the situation is the fabrication of single crystalline Zn$_1-x$Co$_x$O thin films characterized as single domains. This paper investigates PLD techniques of Zn$_1-x$Co$_x$O thin films synthesized by the rapid thermal processor and monitored by In-situ RHEED. Surface morphology and crystallographic characteristic evaluated using AFM and XRD. The magnetization, resistivity, and Hall effect measurements were carried out systematically as a function of Co contents using a QD PPMS. To clarify the electronic structure and the magnetic properties associated with the Co ions in Zn$_1-x$Co$_x$O, we have performed X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism measurements. These results and their implications for the understanding of ferromagnetism in Zn$_1-x$Co$_x$O will be discussed.

S1.00150 Transport Measurements and Synchrotron-Based X-Ray Absorption Spectroscopy of Iron Silicon Germanide Grown by Molecular Beam Epitaxy$^1$, NADER ELMARHOUMI, RYAN COTTIDER, Texas State Univ/Univ of North Texas, GREG MERCHEAN, AMITAVA ROY, CAMD/LSU, CHRIS LOHN, HEIKE GEISLER, CARL VENTRICE JR., TERRY GOLDING — Some of the iron-based metal silicide and germainide phases have been proposed to be direct band gap semiconductors. Therefore, they show promise for use as optoelectronic materials. We have used synchrotron-based x-ray absorption spectroscopy to study the structure of iron silicon germainide films grown by molecular beam epitaxy. A series of Fe(Si$_{1-x}$Ge$_x$)$_2$ thin films (2000 – 8000Å) with a nominal Ge concentration of up to $x = 0.04$ have been grown. X-ray absorption near edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) measurements have been performed on the films. The nearest neighbor coordination corresponding to the $\beta$-FeSe$_2$ phase of iron silicide provides the best fit with the EXAFS data. Temperature dependent (20 $< T < 350$ K) magneto transport measurements were done on the Fe(Si$_{1-x}$Ge$_x$)$_2$ thin films via Van Der Paw (VDP) Hall configuration using a 0.5-T magnetic field and a current of 10-200 μA through indium ohmic contacts. The Hall coefficient was calculated. Results suggest semiconducting behavior of the films which is consistent with the EXAFS result.

$^1$This work was supported by ONR (Contract No. N00014-03-1-0820).

S1.00151 Effect of N to In flux ratio on the InN surface morphologies grown on single crystal ZnO (000T) substrate by plasma-assisted molecular beam epitaxy$^1$, CHENG-HUNG SHIH, IKAI LO, WEN-YUAN PANG, SHIH-HUNG CHUANG, CHIA-HSIUAN HU, Department of physics, National Sun Yat-sen University, Kaohsiung, Taiwan, R.O.C., CHIA-HO HSIEH, Institute of Material Science and Engineering, National Sun Yat-Sen University, Kaohsiung, Taiwan, — The surface morphology of InN epitaxial films grown on ZnO (000T) substrate by plasma-assisted molecular beam epitaxy has been investigated. We found that the evolution of InN surface morphology was sensitive to the N/In flux ratio. With N/In flux ratio decreasing, the growth mode changed from 3D to 2D growth. In addition, we found that In$_n$O$_m$ layer was formed at the interface between InN and ZnO when the N/In flux ratio was lower than 32 by the observation of XRD and TEM.

$^1$The project is supported by National Research Council of Taiwan (NRC 95-2112-M-110-017-MY3) and by AFOSR/AOARD (AFMC, USAF) under grant number FA4607-07-1-0422.

S1.00152 Effect of negatively charged excitons on the phase coherent photorefractive effect in ZnSe quantum wells , A. KABIR, H.P. WAGNER, Department of Physics, University of Cincinnati, Cincinnati, OH 45221, USA — We investigate the effect of negatively charged excitons (trions) on the efficiency and dephasing rate of the phase coherent photorefractive (PCP) effect in ZnSe/Zn$_x$Mg$_{1-x}$Se single quantum wells using 90 fs light pulses. Intensity, temperature and spectrally dependent measurements are performed in a transient four-wave mixing configuration. In the presence of trions the PCP effect is composed of both a fast dephasing component that is caused by the formation of a trion grating and a slower decaying component caused by an exciton grating. With decreasing temperature the trion dephasing rate significantly increases while the exciton dephasing rate remains almost constant. The trion dephasing rate also increases with decreasing barrier width between the ZnSe quantum well (QW) and the GaAs substrate which is attributed to an enhanced electron density of captured substrate electrons in the QW. Model calculations based on the optical Bloch equations are in agreement with the experimentally observed PCP traces.

S1.00153 Effect of annealing temperature of ZnO seed layer on growing aligned ZnO nanorods$^1$, JENN-KAI TSAI, Department of Electronic Engineering, National Formosa University, Yunlin 632, Taiwan, Republic of China, CHU-YU WEI, YI-CHI CHEN, YOU-CHENG HENG, Institute of Electro-Optical and Materials Science, National Formosa University, Yunlin 632, Taiwan, Republic of China, TSEN-HANG MEEN, Department of Electronic Engineering, National Formosa University, Yunlin 632, Taiwan, Republic of China, — Vertical aligned ZnO nanorod arrays were synthesized by hydrothermal method on the Si substrate with a sputtered thin ZnO seed layer on it. Different annealing temperatures of ZnO seed layer were studied in order to understand the ZnO nanorod growth mechanisms. The results show that ZnO nanorods grow faster if the seed layer annealed at higher temperature. The photoluminescence spectra exhibit ultraviolet emission and a broad green emission. The green emission is attributed to the oxygen vacancies in the ZnO nanorods. Further investigations using the scanning electron microscopy, x-ray diffraction, atomic force microscopy were also demonstrated.

$^1$The authors would like to acknowledge financial support from the National Science Council of Republic of China(NSC 97-2112-M-150-002).

S1.00154 High Quality Epitaxial ZnO Films Grown Using Magnetron Sputtering$^1$, TOM ODER, Youngstown State University — Zinc oxide films were sputter-deposited at 500 °C on sapphire. SiC and GaN substrates using different mixtures of Ar and O$_2$. Post-deposition annealing up to 900 °C in N$_2$ with rapid thermal processor resulted in films whose crystalline quality improved with the annealing temperature. The effects of deposition and annealing using different Ar-O$_2$ gas mixtures were also investigated. Films grown on sapphire in a 1:1 Ar-O$_2$ mixture and annealed in N$_2$ at 900 °C for 5 min had the best quality. Room-temperature photoluminescence spectroscopy measurements revealed a near band edge luminescence at 3.5 eV with a FWHM value of 126 meV. The two-theta XRD measurements of these films showed a peak at 34.8°, which corresponds to the diffraction from the (0 0 2) plane of the ZnO and indicates a strong c-axis orientation perpendicular to the surface at the sapphire substrate. Results from the transport properties of these films determined using Hall-effect measurements will be discussed.

$^1$This research was supported by funds from the Research Corporation for Science Advancement.

S1.00155 IR-Dielectric functions of ZnBeTe alloys determined by spectroscopic ellipsometry . NIRJAN MANDAL, FRANK PEIRIS, Physics, Kenyon College, OLEG MAKSIMOV, MARIA TAMARGO, Chemistry, CUNY — Using spectroscopic ellipsimetry, we have determined the complex dielectric function of a series of ZnBeTe II-VI semiconductor alloys between a spectral range of 2000 nm and 40,000 nm. A standard inversion technique was used to obtain the dielectric functions from the measured ellipsimetric spectra. By modeling the dielectric functions as a collection of oscillators, representing longitudinal and transverse optical phonons associated with the ZnBeTe lattice, we were able to recover the phonon spectra for this alloy system. It is argued that the the additional phonon modes that are obtained from ellipsimetry are best understood from the recently-proposed percolation model.
S1.00156 A Method for Determining Refractive Indices of Compound Materials of Epilayers of Multilayer Quantum Structure1,2. GAGIK SHMAVONYAN, State Engineering University of Armenia — A method of determining the refractive indices of compound materials of epilayers of multilayer quantum structures of optoelectronic devices has been suggested. The difficulty with the determination of the refractive indices of the above-mentioned epilayers is that the exactness of the determination of the same parameters of compound materials of epilayers is not high as their values obtained by various methods are quite different. Therefore, the difference between values of bulk and epitaxially grown materials is great. For that reason beam profiles of light emitted from multilayer quantum structure of optoelectronic devices are experimentally investigated and theoretically calculated. The latter allows us to determine the refractive indices of compound epilayers of multilayer active layer of nanostructured optoelectronic devices. As this method consists in the confrontation of theoretical calculations and experimental results, it allows to precisely determine the refractive indices of compound epilayers.

1 Author thanks NATO for FEL.RIG980772 grant.

S1.00157 Synthetic Cu2O crystals with various morphologies prepared by thermal oxidation3. SHAHIN MANI, JOON JANG, JOHN KETTERSON, Department of Physics & Astronomy, Northwestern University, KETTERSON’S TEAM — Cuprous oxide (Cu2O) is an extensively studied semiconductor with a rich history in exciton related physics; it has also been a popular solar cell material. A major impediment to workers studying this material has been the difficulty in fabricating high quality crystals. Achieving a low concentration of impurities and defects is an essential requirement in obtaining increased exciton lifetimes. We have prepared high-quality crystals of Cu2O by an improved thermal oxidation technique. Using this strategy we have formed crystals in various geometries including: i) platelets, ii) cylindrical wires, iii) hollow cylindrical structures, and iv) spheres. The formation of hollow cylindrical structures or tubes of Cu2O by oxidizing copper wires in air is especially surprising. We will discuss photoluminescence experiments involving one- and two-photon excitation and optical absorption measurements at 2 K from the synthetic samples, which in some respects out perform natural (geological) crystals. The more unconventional structures of Cu2O may be utilized to confine excitonic matter or serve as high density exciton-polariton cavities

3Supported by the NSF under grant CCF-03-29957.

S1.00158 Effects of atomic randomness on the band structure calculation of Si1−xGex via density functional theory. MD HOSSAIN, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA, JONATHAN FREUND, HARLEY JOHNSON, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA — Electronic band structure calculations for compound semiconductors are usually performed by averaging fitting parameters using the virtual-crystal-approximation in either the pseudopotential method or the tight binding method. The effect of atomic randomness is completely ignored in such calculations. In this work, without using any fitting parameters, density functional theory is employed to calculate the band structure of the Si1−xGex alloy system taking into account the effect of atomic randomness and, correspondingly, the local strain relaxation. The variation of band gap with 16 different Ge fractions in the alloy is computed to find bowing parameters for the two distinct composition ranges: 0 ≤ x ≤ 0.85 and 0.85 ≤ x ≤ 1.0. The calculation is carried out for a supercell of 64 atoms with P1 symmetry, and the randomly positioned atoms are relaxed up to a force tolerance of 0.0001eV/Å. Our results show much better agreement with experimental results for bandgaps, especially near Si0.85Ge0.15, than available empirical methods do. The results demonstrate the importance of accounting for the effect of randomness and local strain in band structure calculations.

S1.00159 High Yield Microsphere Formation Using an Excimer Laser4. RYAN LU, TERESA EMMERY, AYAX RAMIREZ, SPAWAR Systems Center, Pacific — The need for low-cost photonic devices has stimulated a significant amount of research in silicon photonics. Although silicon photonics is less well-developed as compared to III–V technologies, it has the potential to make a huge impact on the optical communications industry. Silicon is transparent in the standard ITU optical communication bands, which makes silicon the material of choice for passive and active optoelectronic devices. Recently, microspheres are gaining an important place in the optical microcavity resonator community due to their high quality factor morphology-dependent resonances (MDRs). Silicon microspheres with high quality factor morphology dependent resonances are used for resonant detection and filtering of light in the near infrared. The experimentally measured quality factors are limited by the sensitivity of the experimental setup, however, the microsphere quality factor is several magnitudes of order higher than current microring resonators. These optical resonances provides the necessary narrow linewidths, that are needed for high resolution micro-photonic applications. A reproducible process to quickly fabricate uniform microsphere particles with a narrow distribution of diameters and high yield is presented in this paper.

4 Funded by Office of Naval Research.

S1.00160 Nitric-phosphoric acid etching effects on the surface chemical composition of CdTe thin film. IRFAN IRFAN, HUANJUN DING, Department of Physics and Astronomy, University of Rochester, WEI XIA, HAO LIN, CHING W. TANG, Department of Chemical Engineering, University of Rochester, YONGLI GAO, Department of Physics and Astronomy, University of Rochester — Nitric-phosphoric (NP) acid etching has been regarded as one of the most successful methods for the formation of low resistance back contact with the metal electrode in CdTe-based solar cells. We report back surface chemical composition for eight different durations of NP etching of CdTe polycrystalline thin film. We studied the surfaces with x-ray photoemission spectroscopy (XPS), ultraviolet photoemission spectroscopy (UPS), inverse photoemission spectroscopy (IPES) and atomic force microscopy (AFM). Etching dependence on the back surface composition and electronic structure was observed. Valence and conduction band shifts relative to the Fermi level of the system with different etching duration were analyzed. The sample was left in open ambient condition for three weeks and XPS data were obtained again in order to study the difference in surface chemical composition with the pristine CdTe film. Unetched and highly etched part of the sample were sputtered and the depth profile analyzed.

S1.00161 ABSTRACT WITHDRAWN

S1.00162 Elastic strain sharing in silicon nanomembranes from a silicon nitride stressor layer1,2. ANNA CLAUSEN, University of Wisconsin-Madison, DON E. SAVAGE, MAX G. LAGALLY — Strained-silicon (001) nanomembranes have increased electron mobility relative to their unstrained counterparts and are therefore of considerable interest for ultra-fast flexible electronics [1]. The increased mobility is caused by the strain splitting of the delta valleys in the conduction band and the concomitant reduced inter-valley scattering of charge carriers. Previous work using SiGe as the stressor layer on silicon-on-insulator (SOI) requires epitaxial growth and is restricted to tensilely straining Si. We grow polycrystalline SiN on SOI by PECVD to form tensilely as well as compressively strained Si nanomembranes. When the SiN/Si film is released from the buried oxide layer, the strain in the SiN layer is elastically shared with the Si layer. The strain-relaxed nanomembrane is then bonded onto a new substrate. XRD, Raman, and TEM are used to characterize the strain transfer and the presence or absence of dislocations in the Si nanomembrane. Our results are in good agreement with predictions from continuum elasticity theory. [1] Yuan, H-C. et al., Semicond. Sci. Tech. 22, S72-S75 (2007).

1 Supported by the DOE.
S1.00163 Chemical, Electrical and Thermal Characterization of Nanoceramic Silicon Carbide, HERVIE MARTIN, MALEK ABUNAEMEH, CYDALE SMITH, CLAUDIU MUNTELE, SATILMISH BUDAK, DARYUSH ILA, Alabama A&M University — Silicon carbide (SiC) is a lightweight high bandgap semiconductor material that can maintain dimensional and chemical stability in adverse environments and very high temperatures. These properties make it suitable for high temperature thermoelectric converters. At the Center for Irradiation of Materials (CIM) we design, manufacture and fabricate nanoceramic SiC, and perform electrical, thermal and chemical characterization of the material using particle induced X-ray emission (PIXE), Rutherford backscattering spectroscopy (RBS), Seebeck coefficient, electrical conductivity, and thermal conductivity measurements to calculate its efficiency as a thermoelectric generator. We are looking to compare the electrical and thermal properties of SiC ceramics with some other materials used for the same purposes.

S1.00164 Mechanical Properties of Nanoceramic Silicon Carbide, IPIDISO OJO, MALEK ABUNAEMEH, CYDALE SMITH, CLAUDIU MUNTELE, DARYUSH ILA, Alabama A&M University — Generation IV nuclear reactors will use the TRISO fuels, a type of micro fuel particle. It consists of a fuel kernel coated with four layers of isotopic material. One of the materials considered for these layers is silicon carbide ceramic. This lightweight material can maintain chemical and dimensional stability in adverse environments at very high temperatures up to 3000°C, and it is chemically inert. It is widely used as a semiconductor material in electronics because of its high thermo conductivity, high electric field break down strength, and high current density, which makes it more desirable than silicon. Silicon carbide has a very low coefficient of thermal expansion and has no phase transition that would discontinue its thermal expansion. At the Center for Irradiation of Materials (C.I.M.) we are developing a new fabrication process for nanopowdered silicon carbide for TRISO fuel coating purposes. We also study the mechanical properties of the material produced. Among the different test being performed are particle induced X-ray emission (PIXE) an Rutherford backscattering spectroscopy (RBS). The mechanical properties of interest are hardness (measured by Vickers Hardness machine), toughness (measured by the Anistis equation, KIC= 1.6 x 10^-6(E/H)^1/2(P/C0)^5, where P=load, C0=crack length, E=Young’s modulus and H=Vickers Hardness), tensile strength and flexural strength (measured by a three point bend test). Results will be presented during the meeting.

S1.00165 Investigation on Ge induced GaAs(001)-(1x2) structure, JUN NARA, National Institute for Materials Science and IIS, University of Tokyo, AKIHIRO OHTAKE, National Institute for Materials Science, TAKAHISA OHNO, National Institute for Materials Science and IIS, University of Tokyo — It is known that at the initial stage of the Ge growth on GaAs(001), a reconstructed structure with a (1x2) periodicity is formed. A structure model with Ga-Ge dimers on an As-terminated surface has been proposed for the (1x2) reconstruction. On the other hand, the previous studies have shown that As atoms segregate to the growing Ge surface at the initial growth stages. We have reexamined the atomic structure of the Ge-induced (1x2) reconstruction experimentally and theoretically. We show that the initial growth of Ge on GaAs(001) induces the formation of Ga-As dimers as a result of the site exchange between deposited Ge atoms and subsurface As atoms. We confirmed that this atomic geometry is energetically favored compared with the previously proposed Ga-Ge dimer model, by using first-principles calculations. Our proposed structure model accounts well for the experimental results. This work was partly supported by the RISS project in IT program and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government.

S1.00166 Monte Carlo Calculations of the Specific Heat in Quantum Critical Metals, JOHN GADDY, WOUTER MONTFROIJ, University of Missouri - Columbia, THOMAS VOJTA, Missouri University of Science and Technology — Quantum critical magnetic metals have unusual low temperature response such as an anomalous temperature dependence of the electronic specific heat (C0 ∼ T lnT). This dependence originates in the competition between ordering local magnetic moments and the conduction electrons shielding the moments. The Kondo Temperature, T K, when moments become shielded depends on the inter-atomic distances. In most systems that have been investigated experimentally quantum criticality is obtained through lattice expansion by chemical substitution, one can expect a distribution of T K reflecting altered local inter-atomic distances. The random removal of these moments leads to the formation of magnetic clusters in quantum critical metals which has indeed been observed in quantum critical CeRu0.5Fe1.5Ge2. We investigate the dependence of the specific heat through the formation through magnetic cluster formation. Once a cluster separates itself from the lattice, it should order and affect the specific heat. Using a Monte Carlo simulation we calculate the changes in specific heat associated with cluster formation for various Kondo temperature distributions, and we compare our results to those measured in 122-systems like CeRu0.5Fe1.5Ge2.

S1.00167 Study of oxidation of titanium by x-ray photoelectron spectroscopy, HONG DONG, A.R. CHOURASIA, R.L. MILLER, Dept. of Physics, TAMU-Commerce — The oxidation of titanium has been investigated using the technique of x-ray photoelectron spectroscopy. Thick films of titanium have been deposited on silicon substrates by e-beam method. The Oxford Applied Research EGN4 was used for this purpose. The titanium substrate was kept at different temperatures (100, 200, 300, 400, 500, and 600°C). These substrates were exposed to oxygen at different partial pressures. The titanium 2p and oxygen 1s regions have been investigated by XPS. The magnesium anode (energy = 1253.6 eV) has been used for this purpose. The titanium substrate was kept at different temperatures (100, 200, 300, 400, 500, and 600°C). These substrates were exposed to oxygen at different partial pressures. The spectral data have been recorded at 45˚ take-off angle. The spectral data for different temperatures and oxygen partial pressures have been analyzed to ascertain the complete oxidation of the titanium substrate.

S1.00168 Synthesis and characterization of TiO2 nanocrystals through sol-gel and hydrothermal methods, CORINA ILEANA ORHA, CARMEN LAZAU, CORNELIA ELENA RATIU, PAULA SFIRLOAGA, PAULINA VLAZAN, National Institute for Research and Development in Electrochemistry and Condensed Matter Timisoara, Romania, PAUL BARVINSCHI, West University from Timisoara, Romania, IOAN MUSCUTARIU, Physics Department, Baldwin Wallace College, USA, IOAN GROZESCU, National Institute for Research and Development in Electrochemistry and Condensed Matter Timisoara, Romania — Nanomaterials with special and interesting properties, which can be different comparing to the macro scale materials, offer a large area of practical applications in all social-economical fields. Incorporating metallic and non-metallic dopant ions into the titanium dioxide particles can influence the performance of these photocatalysts. This affects the dynamics of electron-ion recombination and interfacial charge transfer. In this paper it was synthesized undoped and doped TiO2 nanocrystals with metallic (Ag) and non-metallic (N) ions through sol-gel and hydrothermal methods. The materials were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDAX), diffuse reflectance UV-VIS, thermogravimetric analysis (TG) and differential thermal analysis (DTA).

S1.00169 Observation of acousto-elastic hysteresis in kinking nonlinear elastic solids, PETER FINKEL, AIGOU ZHOU, MICHEL BARSOUM, Drexel University — Using bulk acoustic waves we studied the nonlinear mechanical properties and hysteresis of the acousto-elastic effect in kinking nonlinear elastic, KNE, solids. The experiments reviewed here present direct observation of nonlinear hysteretic scattering and attenuation of ultrasonic waves in Ti3SiC2 and Ti3AlC2, representatives of KNE solids, as a function of quasi-static cyclic compressive stresses. We attribute this dynamic behavior to the interaction of the acoustic waves with dislocation in incipient kink bands. The relevance of these findings to possible sensor applications of hysteretic KNE solids is briefly discussed.
S1.00170 Spectral Calculations for columnar Thin Films Deposited on Periodically Decorated Substrates, JON MEASE, student, TARIQ GILANI, AKHLESH LAKHTAKIA, Penn State University — Using a morphological model of a class of nano-engineered materials called columnar thin films (CTFs) deposited on periodically decorated substrates, we compute their optical reflection and transmission spectra. The calculation procedure involves the use of the MIT Electromagnetic Equation Propagation (Meep) software libraries. The deposition geometry and the spatial periodicity affect the spectra in technologically significant ways. Our current efforts are focused on a narrowband, linear-polarization rejection filter.

S1.00171 Light reflection from semiconductor surface with submonolayer cover of metal particles, IRINA BARIKAHTAR, Department of Physics, BC, USA, VALERI LOZOVSKI, TATIANA MISHAKOVA, Department of Semiconductor Electronics, KNU, Ukraine — In the framework of the Green function method, the effective susceptibility of submonolayer of metal particles covering the surface of semiconductor is calculated. The main point of calculations is taking into account the size and the shape of the particles. The particles are assumed to have the shape of the ellipse of revolution. The effective susceptibility was obtained in the form: \( \chi(k, \omega) = \left[ \chi^{-1}(k, \omega) - mG_{\text{eff}}(k, \omega) \right]^{-1} \), where \( m \) is the concentration of the particles, \( G_{\text{eff}}(k, \omega) \) is the Green function of the substrate, and \( \chi(k, \omega) \) is the linear response function of the single particle in the surface. Based on this, the exact form of the effective linear response function is calculated. As a result, the reflection coefficient is readily obtained via effective susceptibility and Green function. This approach allows studying the dependence of the reflection coefficient on the particle concentration and its shape, and development of the theory of ellipsometry.

S1.00172 Electronic Properties of Large-scale Graphene Chemical Vapor Synthesized on Nickel and on Sapphire, HELIN CAO, LIYUAN ZHANG, YONG CHEN, Department of Physics and Birck Nanotechnology Center, Purdue University, QINGKAI YU, Department of Electrical and Computer Engineering, University of Houston, HAO LI, Department of Mechanical and Aerospace Engineering, University of Missouri — We have studied the electronic transport properties of large area few-layer graphene/graphitic films grown by two different chemical vapor based methods. The first type of samples (metal-transfer graphene) is synthesized by carbon segregation from Ni, then transferred to SiO2/Si substrates. The second type of samples is synthesized by direct chemical vapor deposition (CVD) on sapphire. We measured these samples under variable temperatures (from 2K to 300 K) and transverse magnet fields (from 0 to 7 T). For both types of samples, we found a negative magnetoresistance at low field, and carrier mobilities on the order of several hundreds of cm²/V-s. For metal-transfer graphene, in particular, we were able to measure a moderate field effect response, using the highly doped Si substrate as back gate. The observed magnetoresistance shows characteristic features of weak localization, from which we extract various scattering lengths in the metal-transfer graphene samples. Comparison with those measured in mechanically exfoliated graphene suggests possibly different carrier scattering mechanisms for graphene materials prepared with different methods.

S1.00173 All-electron KKR Calculations for Metallic Systems with Thousands of Atoms Per Cell via Sparse Matrix Iterative Solvers, SUFFIAN KHAN, AFTAB ALAM, DUANE JOHNSON, University of Illinois at Urbana Champaign — To perform electronic-structure calculations for inherently large systems, such as a quantum dots or interfaces like domain walls, we must perform the calculations over very large unit cells (10⁵ to 10⁶ atoms). For the inverse Green’s function \( G^{-1} \), KKR methods typically solve for \( G \) by direct inversion. Using a screened, k-space hybrid KKR, we solve Dyson’s equation for the Green’s function using a reference state via \( G = G_{\text{ref}} \). For both types of samples, we found a negative magnetoresistance at low field, and carrier mobilities on the order of several hundreds of cm²/V-s. For metal-transfer graphene, in particular, we were able to measure a moderate field effect response, using the highly doped Si substrate as back gate. The observed magnetoresistance shows characteristic features of weak localization, from which we extract various scattering lengths in the metal-transfer graphene samples. Comparison with those measured in mechanically exfoliated graphene suggests possibly different carrier scattering mechanisms for graphene materials prepared with different methods.

S1.00174 Many-flavor electron gas approach to electron-hole drops, GARETH CONDUIT, University of Cambridge, PETER HAYNES, Imperial College — A many-flavor electron gas (MPEG) is analyzed, such as could be found in a multivalley semiconductor or semimetal. Using the rederived polarizability for the MPEG, an exact expression for the total energy of a uniform MPEG in the many-flavor approximation is found. The interacting energy per particle is shown to be \( -0.574447 \left( E_0 a_0^2 \right) \left( m^* \right)^{1/2} \left( m^* \right)^{1/2} \left( m^* \right)^{1/2} \), with \( E_0 \) being the Hartree energy, \( a_0 \) being the Bohr radius, and \( m^* \) being the effective mass. The short characteristic length scale of the MPEG motivates a local-density approximation, allowing a gradient expansion in the energy density and the expansion scheme is applied to electron-hole drops, finding a new form for the density profile and its surface scaling properties. The formalism is verified using both Quantum Monte Carlo and density-functional theory calculations.

S1.00175 3D Quantum Dot Density of States in a Magnetic Field, N.J.M. HORING, Stevens Institute of Technology, Hoboken, USA, S.Y. LIU, Shanghai Jiaotong University, Shanghai, China, V. FESSATIDIS, Fordham University, Bronx, USA — We have analyzed the detailed quantum dynamics of a 3D magnetic dot in a magnetic field. The dot is taken to be lodged in a bulk medium in a high magnetic field and it is represented by a three-dimensional Dirac delta function potential which would support just one subband state if there were no magnetic field. The integral equation for the retarded Green’s function of this system is solved in closed form analytically and the single particle subband energy spectrum and the density of states are examined taking account of splintering of the subband spectrum by Landau quantization.

S1.00176 SUPPLEMENTARY ABSTRACTS —

S1.00177 Boron-catalyzed growth of multi-wall carbon nanotubes and their mechanical properties, FUMIO KOKAI, TAKASHI OKADA, IORI NOZAKI, AKIRA KOSHIO, Mie University, TORU KUZUMAKI, Tokai University — Carbon nanotubes have received widespread interests in basic and applied research fields. However, many applications of carbon nanotubes are hindered by a lack of control of their precise morphology and microstructures. We report here an efficient synthesis of multi-wall carbon nanotubes (MWNWs) by laser vaporization in inert gas atmosphere. We used a continuous-wave Nd:YAG laser (600 kW peak power) to irradiate a graphite target containing boron carbide (boron content: 1-60 at.%). Young’s moduli of MWNWs were also measured by nanoprobe manipulation in a TEM. The modulus was 680 GPa for a MWN produced in 0.1 MPa Ar for 20 at.% boron content, which is much higher than those (~0.1 GPa) of MWNWs grown by CVD.
S1.00178 How Mass Changes with Velocity and Energy? . LIANGXI MA, Blinn College — It is well known that mass of an object $m$ can increase with its speed $v$, which is one reason that we believe that the speed of light $c$ is the ultimate limit for all objects. As the $v$ is approaching to the speed of light, the $m$ becomes larger and larger so the acceleration becomes more and more difficult. It is also well known that $m$ is related to the energy $E$. Energy is released in the nuclear reaction while the mass is lost and this has been the theoretical basis for nuclear fission and fusion reactions. However, argument exists over how to interpret the relationship between mass and velocity and energy. In the text, we don’t want to discuss if the use of relativistic mass is appropriate. Instead, we discuss two examples that seem to be confusing in the teaching of special relativity. A harmonic spring oscillator and a proton accelerated in an electric field are chosen as examples to discuss the mass change with energy and velocity. We show that the two equations $m = \gamma m_0$ and $m = \frac{mc^2}{\sqrt{1-v^2}}$ agree each other if potential energy and related mass are properly considered.

S1.00179 Manipulation of thermal emission via gold gratings. JONES TSZ-KAI WAN, Department of Physics, The Chinese University of Hong Kong — The photon density of states of a structured metallic surface is strongly modified by various plasmonic excitations; as a result, thermal emission of photons can be manipulated through the control of plasmonic excitations. In this work, the author studies the emission properties of gold gratings, and investigates the effects due to the groove depth and periodicity. By systematically increasing the groove depth, the polarization of the emitted photons can be controlled. In addition emission at particular frequencies could be tuned to achieve that of the blackbody radiation limit, whereas the emission in other frequency ranges does not have noticeable changes.

This work is supported by RGC-HK (GRF project no. 403308) and by the NHMFL.

S1.00180 Absorption spectrum of the Single Molecule Magnet [Ni(dbm)(MeOH)Cl]$_4$. DANIEL J. ARENAS, DAMIETRIOUS KOKUS, SATI ATATA, CHAO CAO, HAI-PING CHENG, DAVID B. TANNER, Department of Physics, University of Florida, STEPHEN HILL, Department of Physics, Florida State University, CHRISTOPHER BEEDLE, DAVID HENDRICKSON, Department of Chemistry and Biochemistry, University of California at San Diego — The room temperature optical absorption of the single-molecule magnet [Ni(dbm)(MeOH)Cl]$_4$ has been measured in the near-infrared-visible spectral region. The spectra show a strong absorption band around 3 eV and bands characteristic of d-d transitions in nickel. The results will be compared to various theoretical models in the literature; including DFT and DFT+U calculations [Phys. Rev. Lett. 100, 167206] that predict different energy gaps for the HOMO to LUMO optical transitions.

S1.00182 BioCARS: A State-of-the-Art Facility for Time-resolved Crystallography with 100ps Time Resolution. ROBERT HENNING, TIM GRABER, VUKICA SRAJER, YU-SHENG CHEN, ZHONG REN, University of Chicago, FRIEDRICH SCHOTTE, PHILIP ANFINRUD, National Institutes of Health, KEITH MOFFAT, University of Chicago — BioCARS, a national facility located at the Advanced Photon Source (APS), recently upgraded the undulator beamline (14-ID) to become one of the best facilities in the world for conducting experiments with SChOTTe, PHILIP ANFINRUD, National Institutes of Health, KEITH MOFFAT, University of Chicago — BioCARS, a national facility located at the Advanced Sample Position.

S1.00183 Raman spectroscopy measurement of MoS$_2$ to 43 GPa. YANZHANG MA, Texas Tech University, BOHENG MA, Thomas S. Wootton High School, HONGYANG ZHU, MING CHYU, Texas Tech University — MoS$_2$ has a typical layered crystal structure. The two-dimensional lattice vibration, in conjunction with the strong (ionic) and weak (Van de Waals) bonding, is a very interesting subject. Among many of the interesting properties of MoS$_2$ is the physical performance in response to the substantial reduction of distance between the layers of the MoS$_2$ network along with the increase of interaction between them. We compressed MoS$_2$ in a diamond anvil cell to 43 GPa and carried out in situ Raman spectroscopy measurement. We found that the vibration energy of the A$_1g$ and E$_g$ modes was elevated with increasing pressure. At about 27 GPa, the peak of E$_g$ mode split into two peaks while the A$_1g$ peak did not show any abnormality. We believe that this reflects a structural phase transformation due to a minimal distortion of the MoS$_2$ network within the layer. We also found that non-hydrostatic compression on the sample lowered the pressure-induced energy elevation of the vibration modes, indicating that the differential stress applied on a MoS$_2$ crystal resists the atomic vibration.

This work is supported by NSF grant number: DMR0619215.

S1.00184 MgB$_2$ under pressure; band-filling, phonon hardening and electrical anisotropy. JESUS VAZQUEZ, SABINA RUIZ-CHAVARRIA, PABLO DE LA MORA, Fac. de Ciencias, Universidad Nacional Autonoma de Mexico — The electrical two-dimensional characteristic has been accepted as an important factor in the high T$_c$ superconductors. In MgB$_2$, it is the almost two dimensional $\sigma$-bands that are responsible for the superconductivity. On the other hand in MgB$_2$, the band-filling and phonon hardening have been found to be the responsible for the high T$_c$. [1] But previous calculations have shown that with pressure both, electrical anisotropy and T$_c$ are reduced. Thus the question arises: Is the electrical anisotropy, together with band-filling and phonon hardening, also responsible of the high T$_c$ in MgB$_2$? Using the WIEN2k package the MgB$_2$ superconductor is analyzed as function of pressure. At each pressure the cell parameters are optimized and the $\sigma$-DOS are calculated and, with the use of the Hopfield expression, are analyzed to see what the correlation of these elements with T$_c$ is. [1] J Kortus, Physica C 456 (2007) 54-62 [2] U Esteves and P de la Mora, Rev. Mex. Fis. 53 (2007) 95-98

S1.00185 ABSTRACT WITHDRAWN

S1.00186 Magnetic properties of Sr$_2$IrO$_4$ a DFT study. PABLO DE LA MORA, Fac. de Ciencias, CARLOS COSIO-CASTANEDA, GUSTAVO TAVIZON, Fac. de Quimica, Universidad Nacional Autonoma de Mexico — Sr$_2$IrO$_4$ is a magnetic insulator with a small Ir-magnetic moment [1]. IrO$_6$ rotations (due to the $I4/mcm$ space group) allow non-collinear magnetic ordering, thus this material could have weak ferromagnetism (non-collinear antiferromagnetically ordered $1\bar{r}$ magnetic moments); other possible explanation is band-magnetism. Simple DFT calculations give a non-magnetic conductor. Intra-atomic electron repulsion can generate magnetic moments in the $d$-orbitals (via the Hubbard $U$ ($U_{ij}$)), but due to extended character of these 5$d$-orbitals the $U_{ij}$ should be quite small. Sr$_2$IrO$_4$ is analyzed with the WIEN2k package. Different magnetic configurations with varying $U_{ij}$ are calculated in order to try to explain the observed magnetic behaviour. [1] C Cosio-Castaneda, G Tavizón, A Baeza and R Escudero, J. Phys.: Cond. Matter 19 (2007) 446210
S1.00187 Magnetic behaviour of the $\text{Bi}_{2-x}\text{Sr}_x\text{Ir}_2\text{O}_7$ pyrochlore. CARLOS COSIO-CASTANEDA, GUSTAVO TAVILON, Fac. Química, PABLO DE LA MORA, Fac. de Ciencias, FRANCISCO MORALES, ROBERTO ESCUDEIRO, Inst. de Materiales, Universidad Nacional Autonoma de Mexico — Polycrystalline compounds of the $\text{Bi}_{2-x}\text{Sr}_x\text{Ir}_2\text{O}_7$ solid solution have been synthesized. These compounds were obtained by the solid state reaction method in the 0 < x < 0.9 range with the α-pyrochlore crystal structure. This material was characterized with X-ray photoelectron spectroscopy and cyclic voltammetry. These analyses permitted the understanding of the unit-cell modifications and valence states of Iridium as a function of the stontent content. Electrical characterization of samples in the 10-300K range shows a metallic character that remains for the whole solid solution. Magnetically this system behaves as a Curie-Weiss paramagnetic in the 2-300K range. The measured magnetic moment values suggest the presence of $\text{Ir}^{5+}$ in some compounds of the solid solution.

S1.00188 Phase behavior of colloid-polymer mixtures in two-dimensions, AMIR AMINI, MARC ROBERT, Rice University — Phase behavior of mixtures of colloidal particles and non-adsorbing polymer chains bounded to two dimensions with various polymer-to-colloid size ratios are investigated. Mixtures are trapped at the air-water interface and pressure-area isotherms are obtained using the Langmuir-Blodgett technique. Different regions of the phase diagram are explored by changing temperature and the concentration of the colloid and the polymer. Brewster angle microscopy is then used to identify the microstructure of the formed phases.

S1.00189 How Local Anesthetics affect the structural and dynamical properties of biomembranes, ZHENGLI YI, Indiana University, MICHIHIRO NAGAO, Indiana University Cyclotron Facility, DOBRIN BOSSEV, Indiana University — To address the question of how local anesthetics influences the structural and dynamical properties of bio-membranes, neutron-spin echo spectroscopy (NSE) has been performed on 1,2-Dimyristoyl-sn-Glycerol-3-Phosphocholine (DMPC) unilamellar vesicles (ULV) with different concentrations of Lidocaine in D2O to study the influence of Lidocaine on the bending elasticity of DMPC ULV bilayers in fluid crystal (Lα) phase and the ripple gel (Pβ1) phase. The measurement of small-angle neutron scattering (SANS) has been performed to determine the bilayer thickness as a function of the concentration of Lidocaine. In the existence of molecules of Lidocaine the bending elasticity of DMPC bilayers was increased 30% -100% in Lα phase. The NSE data confirmed that fluid crystal/ripple gel transition temperature of DMPC bilayers was depressed by the addition of local anesthetics, which has also been examined via differential scanning calorimetry (DSC).

S1.00190 Landau-Zener Interference in Multilevel Superconducting Flux Qubits Driven by Strong Fields, YANG YU, XUEDA WEN, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — We proposed a model to investigate the Landau-Zener (LZ) interference in multilevel superconducting flux qubits driven by large-amplitude microwave fields. The calculated interference patterns agree remarkably with those of the experiments. Moreover, the interference depends on the driving-frequency and dephasing rate. The dephasing generally destroys the interference while increasing frequency rebuilds the interference at large dephasing rate. At certain driving frequency and dephasing rate, the interference shows some anomalous features as observed in recent experiments. Our results can be used to understand the LZ interference in multilevel quantum systems under different driving frequencies and decohore rates.

S1.00191 A Logic-Based Technique that Charaterizes the Class of Boolean Networks Producing a Given Biological Pathway, GUANYU WANG, CHEN ZENG, George Washington University — A central theme in biophysics is the relationship between structure and function. The question becomes especially intricate at the systems level in which the objects of study are biological networks composed of large numbers of interacting molecules. To what extent does the requirement of carrying out a specific function constrain the structural and more general dynamical properties of a network? Does the biological network optimally designed? Here we present an efficient logic-based technique that captures the ensemble of all the networks that realize the same biological function. The biological function is first represented by a dynamical trajectory in the state space, and our first principle simulations on Au/MgO/Au and Pt/MgO/Pt nanocapacitors, we construct an analytical model that isolates the contributions of various physical mechanisms to the intrinsic dead layer. In particular we evidence even in “perfectly” fabricated structures. The exact nature of the intrinsic dead-layer and the reasons for its origin still remain somewhat unclear. Based on insights gained from recently published ab initio work on SrRuO3/SrTiO3/SrRuO3 and our first principle simulations on Au/MgO/Au and Pt/MgO/Pt nanocapacitors, we construct an analytical model that isolates the contributions of various physical mechanisms to the intrinsic dead layer. In particular we argue that strain-gradients automatically arise in very thin films even in complete absence of external strain inducers and, due to flexoelectric coupling, are dominant contributors to the dead layer effect.

S1.00192 Controlling the spatial correlation of entangled photon states using engineered crystal patterns, S.N. ZHU, X.Q. YU, P. XU, Department of Physics, Nanjing University — In this work, we will illustrate a scheme to tailor and manipulate the entangled photon state's spatial mode. When a 532 nm laser is directed on the crystal, it can split the 532nm photon into two degenerate 1064 nm photons. They must be entangled and the structural information in periodic crystal patterns would be transferred into their spatial mode. We performed a far-field interference experiment with such entangled photon pairs. The coincidence count shows a multi-beam two-photon sub-wavelength interference pattern. Our results can be used to control the LZ interference in multilevel quantum systems under different driving frequencies and decoherence rates.

S1.00193 Flexoelectricity in nanostructures and ramifications for the dead-layer effect in nanocapacitors and “giant” piezoelectricity. RAVEI MARANGANTI, University of Houston, MOHAMED MAJDUB, PRADEEP SHARMA, University of Houston — Thin films of high-permittivity dielectrics are considered ideal candidates for realizing high charge density nanoscale capacitors for use in next generation energy storage and nanoelectronics applications. The experimentally observed capacitance of such film nanocapacitors is, however, an order of magnitude lower than expected. This dramatic drop in capacitance is attributed to the so-called “dead layer” — a low-permittivity layer at the metal-dielectric interface in series with the high-permittivity dielectric. Recent evidence suggests that this effect is intrinsic in the sense that its emergence is evident even in “perfectly” fabricated structures. The exact nature of the intrinsic dead-layer and the reasons for its origin still remain somewhat unclear. Based on insights gained from recently published ab initio work on SrRuO3/SrTiO3/SrRuO3 and our first principle simulations on Au/MgO/Au and Pt/MgO/Pt nanocapacitors, we construct an analytical model that isolates the contributions of various physical mechanisms to the intrinsic dead layer. In particular we argue that strain-gradients automatically arise in very thin films even in complete absence of external strain inducers and, due to flexoelectric coupling, are dominant contributors to the dead layer effect.

S1.00194 ABSTRACT WITHDRAWN —
S1.00195 NaCl and Cationic lipid bilayer dynamics. MARKUS S. MIETTINEN, Department of Applied Physics, Helsinki University of Technology, Finland, ANDREY A. GURTVOVENKO, Institute of Pharmaceutical Innovation, University of Bradford, UK, ILPO VATTULAINEN, Department of Physics, Tampere University of Technology, Finland, MIKKO KARTTUNEN, Department of Applied Mathematics, University of Western Ontario, Canada — Positively charged lipid bilayer systems hold promise for safer and more efficient gene and drug delivery. Here we studied cationic bilayers comprising binary mixtures of cationic dimyristoylphosphatidylcholine (DMPC) and zwitterionic dimyristoylphosphatidylglycerol (DMPC) lipids. Using molecular dynamics simulations we addressed the effects of bilayer composition (cationic to zwitterionic lipid fraction) and NaCl electrolyte concentration on the dynamical properties of these systems. We found that despite the DMPC lipids form complexes via Na⁺ ions that bind to the lipid carbonyl oxygens, NaCl concentration had a rather minute effect on the lipid diffusion. The residence times of sodium ions in the carbonyl region appeared to lack a characteristic time scale, although observed a simulation period of over 200 ns. These prolonged dynamics of the sodium ions could be interesting for the physics of the whole membrane, especially to its interaction dynamics with charged macromolecular surfaces. 1. A. A. Gurtovenko et al., J. Phys. Chem. B 109, 21126 (2005) 2. M. Miitinen et al., J. Phys. Chem. B, (submitted)

S1.00196 Achieving quantum-like interference in ostensibly “classical” systems through closed timelike curves, M.J. RAVE, Western Carolina University — It was recently shown [1] that quantum interference can be understood heuristically as a quasi-probability effect as opposed to being interference in the traditional sense. Surprisingly, this interpretation requires one to think of closed loops in time (represented by products of probability amplitudes) as fundamental quantum entities, much as we think of state vectors normally. (These entities, incidentally, share similarities to Berry’s geometric phase.) The question naturally arises: can this closed-loop paradigm elucidate QI, making its idiosyncrasies more mundane? We show that this new way of thinking about QI leads to a whole new class of “classical” systems and analogies that exhibit pseudo-QI effects.


S1.00197 Crack branching and viscous fingering at nanoscale in brittle material. DEEDER AURONGZEB, University of Maryland, James A. Clark School of Engineering, College Park, MD — Cracked surfaces of soda lime glass and single crystal silicon are studied using atomic force microscopy simply by breaking them with impulsive force. We find traces of cavities and reorganized surface structures in both surfaces. At micron scale fractured glass surface exhibits viscous fingering and fractured silicon surface exhibit nanoscale crack branching showing two materials responds to sudden fracture differently. Crack branched surface of Si shows unusually low self-affine exponent and faceted nanoscale organized islands.

S1.00198 Raman spectroscopic studies of monoclinic Gallium Oxide (β-Ga₂O₃) Nanostructures: A comparison between nanowires vs. nanobelts, AURANGZEB KHAN, University of Peshawar, Peshawar Pakistan and Department of Physics & Astronomy and CMSS program, Ohio University, Athens OH 45701, SAIMA KHAN, Department of Civil Engineering, Ohio University, Athens OH 45701, WOJCIECH JADWISIENCZAK, School of Electrical Engineering and Computer Science, Ohio University, Athens OH 45701, MARTIN KORDESCH, Department of Physics and Astronomy and CMSS program, Ohio University, Athens OH 45701, OHIO GROUP TEAM, ELECTRICAL ENGG GROUP COLLABORATION — Nanostructures of monoclinic gallium oxide (β-Ga₂O₃), nanowires and nanobelts were synthesized via a very simple thermal evaporation process by using Ga metallic ignots and β-Ga₂O₃ powder as source materials for gallium and oxygen, respectively. The structural properties of the as grown nanostructures were characterized by using SEM, XRD and EDS. Raman studies were also performed for the grown nanostructures and Raman shifts were compared with the LDA calculated values of the peaks as well as with their bulk counterpart which exhibited good agreements with most of the peaks for both the nanostructures. In addition to this, there are some more Raman shifts which are the characteristics of the nanostructures as they have larger surface to volume ratio compared to their bulk counterparts.

S1.00199 Surface Effects on Amyloid Fibril Formation¹. BRAD MOORES, Department of Physics and Astronomy, University of Waterloo, JANET SIMONS, Department of Biology, University of Waterloo, ZOYA LEONENKO, Department of Physics and Astronomy, Department of Biology, University of Waterloo — Amyloid fibrils are insoluble aggregates composed of proteins in beta-sheet conformation, which are implicated in at least 20 diseases for which no cure is currently available. Although fibril plaque formation is associated with biological membranes in vivo, most of earlier research on fibrillogenesis has been performed in a solution phase, in which only a protein-protein interactions are considered. On the other hand, the surface of plasma membrane could provide the environment in which amyloid forming proteins could cluster. In order to get an insight into the understanding of the effect of the surface of plasma membrane, and the surfaces in general, on amyloid fibril formation, we used Atomic force microscopy to study binding of amyloid beta 1-42 peptide and amyloid fibril formation on model surfaces, such as chemically modified positively charged, negatively charged and hydrophobic substrates. The results show that structure, size and amount of larger fibrils and smaller aggregates depend on the type of surface, and differ from aggregation observed in solution.

¹Supported by Natural Science and Engineering Research Council of Canada.

S1.00200 High Resolution TEM Imaging of Graphene by use of aberration-free microscope, R005 , TAKAYUKI TANAKA, Tokyo Institute of Technology, CREST-JST, YUUSUKE ABE, Tokyo Institute of Technology, HIDETAKA SAWADA, EJJI OKUNISHI, YUKIHITO KONDO, JEOL, CREST-JST, KUNIO TAKAYANAGI, Tokyo Institute of Technology, CREST-JST — Free-standing Graphene is imaged by use of a novel transmission electron microscope (TEM), R005, equipped with newly-designed Cs Correctors for TEM and STEM. The R005 microscope is fitted with 300kV cold-field emission gun (CFEG) to minimize the chromatic aberration, resulting in achievement of 50pm resolution. Its high phase contrast allows direct imaging of graphene without image reconstruction. The TEM Image of graphene can be distinguished from that of graphite and confirmed by simulation. The adatoms and defects of single carbon atom, which cause the modulation of electronic properties, are also observed.

S1.00201 Affordable Integrated Technology Projects Science Education towards New Horizons. FRANCO PAOLETTI, East Windsor Regional School District, East Windsor, NJ, LISA MARIE CARLUCCI, Global Education & Research, Princeton, NJ — The new-era concept of education supports a type of instruction whereby technology directly acts as a conduit of change, fundamentally altering what is learned, how it is learned, and the role of the educator in the classroom. In our current world, the learning about technology itself has become a goal and a means to successful participation in today’s society. Efficient integration of technology to enhance and support the educational process will: 1) provide educators with the resources and the freedom to actualize innovative educational programs; 2) allow educators to be successful in challenging each student to reach his/her highest potential to ultimately increase academic achievement. This study analyzes what technology integration into education means identifying the benefits and the challenges that educators need to meet in order to be successful in their efforts while providing examples of how to successfully implement effective programs under budgetary constraints.
S1.00202 In-situ High Resolution TEM Observation of Dynamic Structural Changes of Au/TiO2 Catalyst Exposed to Oxygen and Hydrogen, KENTARO SANO, Tokyo Institute of Technology, TAKAYUKI TANAKA, Tokyo Institute of Technology, CREST-JST, HIDETAKA SATANADA, YUKIHIRO KONO, JEOL, KUNIO TAKAYANAGI, Tokyo Institute of Technology, CREST-JST. — Recently atomic structures of Au nanoparticles (NPs)/TiO2 catalyst are discussed in relation to its high catalytic activity. In addition, the importance of in-situ experiments in gas environments has increased. We have developed a novel gas-injection holder, which allows in-situ observations at high pressures up to 100 Pa. We observed Au NPs on TiO2 exposed to gas including oxygen and hydrogen. The exposure to oxygen induced growth of buffer layer on TiO2 surface. The buffer layer attached Au NPs and often covered Au NPs. The growth of buffer layer has not been reported so far, while it appears to cause the substrate roughening. These results suggest the importance of disorder phenomena in the transition layers. The EELS experiments suggest that the buffer layer is highly oxidized titania. On the contrary the exposure to hydrogen induce a slight change of TiO2 surface and remarkable changes of Au NPs morphology. These in-situ observations greatly contribute the clarification of catalysis of Au NPs/TiO2.

S1.00203 Upper bounds on photonic bandgaps in two and three dimensions, MIKAEL RECHTMAN, Courant Institute, NYU, SALVATORE TORQUATO, Princeton University — A 20-year search has been on to find photonic crystals (periodic dielectric structures) with the largest possible full photonic bandgaps. A large robust bandgap is key to the many applications of these materials, which include near-lossless waveguiding, optical filtering, optical computing, and others. A number of three-dimensional structures with large gaps have been proposed (e.g., a diamond lattice of spheres [1], the “Woodpile” structure [2], and in two dimensions, structural optimizations to find the largest-bandgap structure have been performed, e.g., [3], [4]). So far, however, there has been no work on finding rigorous limits on how high the bandgap may be. In this talk, I present upper bounds on the bandgaps of two- and three-dimensional photonic crystals.

1 This research was supported by grant DC00241 from the National Institutes of Health. AJH is an Investigator of Howard Hughes Medical Institute.

S1.00204 Anomalous Brownian motion and viscoelasticity of the ear’s mechanoelectrical transducer, DANIEL ANDOR-ARDÓ, ANDREI KOZLOV, A.J. HUDSPETH, The Rockefeller University — The Brownian motion of a particle in a complex environment is known to display anomalous power-law scaling in which the mean squared displacement is proportional to a fractional power of time. Using laser interferometry and analytical methods of microhemeology, we examine nanometer-scale thermal motions of hair bundles in the internal ear and show that these cellular organelles undergo fractional Brownian motion. This anomalous scaling is caused by viscoelasticity of the gating springs, elements that transmit energy in a sound to the mechanosensitive ion channels. These results demonstrate a connection between rheology and auditory physiology, and indicate that statistical properties of the thermal noise in the ear can be determined by dynamics of a small number of key molecules.

S1.00205 ABSTRACT WITHDRAWN

S1.00206 ABSTRACT WITHDRAWN

S1.00207 Label-free detection of DNA interactions by terahertz spectrometry, ANIS RAHMAN, Applied Research and Photonics, Inc., BRUCE STANLEY, Penn State College of Medicine, AUNIK RAHMAN, Applied Research and Photonics, Inc., ARP TEAM — Terahertz (THz) spectrometry has the potential to analyze DNA and other molecular interactions without fluorescent labeling. THz spectrometry is conducted in time domain where the temporal signal is acquired on a sub-pico-second scale. The temporal signal converted to frequency domain via Fourier transform constitutes a signature of the interaction under study. An important advantage of this technique is that the delay time can be tuned from tens of femto-seconds to tens of pico-seconds. This gives a means of probing a molecular “event” (e.g., a vibrational state or bond position or bending, or a conformational state, etc.) in an appropriate time window. This is a powerful ability because different molecular events exhibit different time response based on their physical and chemical nature. For example, a molecular relaxation occurs over a longer time scale compared to a bond vibration. Similarly, compositional or conformational difference of a given molecule results in different signature with appropriate time response that can be accurately probed. The terahertz signature is unique and provides a means of identifying and/or characterizing many molecular interactions. Some exemplary results of biological system will be discussed.

S1.00208 Void collapse in energetic structural materials, DEREK REDING, SATHYA HANAGUD, Georgia Institute of Technology — A spherically symmetric pore collapse model is introduced that incorporates internal and physical state variable plasticity models for a mixture. This model is based on the modified Carroll-Holt model by Nesterenko. Mixture rules are formulated for the density and yield strength. Previous spherically symmetric model studies consider single constituent porous mixtures. This study investigates the pore collapse in the Ni+Al − void system during shock loading. This material is part of a larger class of energetic structural materials. The proposed model is incorporated into a gas-gun simulation via an algorithm that uses the bisection method for robustness. Results show close agreement between simulation and experiments for shock pressures up to 6 GPa. The proposed mixture pore collapse model is useful for incorporation into a continuum level simulation of the gas-gun experiment.

This research was funded by the AFOSR MURI 1606U81 on Multifunctional Energetic Structural Materials at the Georgia Institute of Technology.

S1.00209 Evidence for a disorder-phase transition in the condensation of 4He in aerogels, FABIEN BONNET, MATHIEU MELICH, LAURENT PUECH, PIERRE ETIENNE WOLF, Institut Néel CNRS-UJF — Although widely studied, capillary condensation of fluids in disordered mesoporous media is not fully understood. A central question is the origin of the hysteretic behavior between adsorption and desorption. It has been recently proposed that this hysteresis could result from the disorder of the porous media. Based on mean-field theoretical calculations, a disorder-driven transition is predicted, similar to that occurring in the Random Field Ising Model. Our earlier results on the condensation of helium in silica aerogel, combining thermodynamic (adsorption isotherms) and optical measurements, have provided a first evidence for such a transition. Here, we report new measurements on aerogels (porosity: 95%, 97% and 98.5%), which further support the disorder scenario, and allow us to study the interplay between temperature and disorder. We also compare the case of aerogels to that of Vycor. Although a transition is not observed in Vycor, the dynamics of the adsorption and desorption processes lead us to conclude that disorder is also important in this case. F. Bonnet et al. Europhys. Lett. 82, 56003 (2008)
S1.0021 Ambient Detection of Energetic Materials by Matrix Assisted Laser Desorption and Photofragmentation-Fragment Detection. STEPHEN ROBERSON, ROSARIO SAUSA, US Army Research Laboratory — We detect energetic materials TNT and RDX by Matrix Assisted Laser Desorption (MALD) followed by photofragmentation-fragment detection (PF-FD) in real time at ambient conditions. A pump laser irradiates a mixture of energetic material and laser dye freeing the energetic material from the surface, and a second laser fragments the resulting energetic molecule to create the characteristic nitric oxide (NO) fragment, which is subsequently ionized and then detected by resonance-enhanced multiphoton ionization (REMPI). Our studies on the effects of pump and probe laser energy, dye concentration, and analyte concentration on the ion signal intensity, as well as the RDX and TNT limits of detection will be reported at the meeting. The PF-FD technique exhibits great potential for detecting trace energetic materials on surfaces because of its high sensitivity and selectivity. It is not restricted to TNT and RDX, and can be extended to other energetic materials.

1National Research Council Postdoctoral Research Associate

S1.00211 Molecular dynamics simulations of electrostatics and hydration distributions around RNA and DNA motifs. ASHLEY E. MARLOWE, ABHISHEK SINGH, ANDREY V. SEMICHAEVSKY, YAROSLAVA G. YINGLING, North Carolina State University, MATERIALS SCIENCE AND ENGINEERING TEAM — Nucleic acid nanoparticles can self-assemble through the formation of complementary loop-loop interactions or stem-stem interactions. Presence and concentration of ions can significantly affect the self-assembly process and the stability of the nanostructure. In this presentation we use explicit molecular dynamics simulations to examine the variations in cationic distributions and hydration environment around DNA and RNA helices and loop-loop interactions. Our simulations show that the potassium and sodium ionic distributions are different around RNA and DNA motifs which could be indicative of ion mediated relative stability of loop-loop complexes. Moreover in RNA loop-loop motifs ions are consistently present and exchanged through a distinct electrogentic channel. We will also show how we used the specific RNA loop-loop motif to design a RNA hexagonal nanoparticle.

S1.00212 Disentanglement and Re-entanglement of Polymer Solutions after Large Step Shear Deformation. YANGYANG WANG, SHI-QING WANG, University of Akron — Double-step strain and elastic recovery experiments were carried out to explore the disentanglement and re-entanglement kinetics in entangled 1,4-polybutadiene solutions after large step shear deformation. In double-step strain experiments, startup shear measurements were interrupted at different strains, and resumed after different waiting times. When the interrupted strain was small, the magnitude of stress overshoot in the resumed shear remained unchanged. However, at a large strain, the magnitude of stress overshoot would first decrease with increasing waiting time and then only become higher after longer waiting time. This observation reveals evidence that disentanglement occurs after a large step deformation. Subsequent healing in the form of re-entanglement allows the sample to relax normally in quiescence. In elastic recovery experiments, the data at small strains fall onto a master-curve, whereas the recovery at large strains shows much stronger strain dependence, confirming occurrence of chain disentanglement beyond a critical strain amplitude.

S1.00213 Phonons in strongly correlated materials from Hubbard-corrected density-functional-perturbation theory. ANDREA FLORIS, Institut für Theoretische Physik, Freie Universität Berlin, Germany and European Theoretical Spectroscopy Facility (ETSF), MATTEO COCCOCCIONI, Chemical Engineering and Materials Science Department, University of Minnesota, Minneapolis, USA — A novel DFT+U energy functional (named DFT+-U-V) is introduced based on a corrective Hubbard Hamiltonian that includes both on-site (U) and inter-site (V) electron-electron interactions. The competition between these couplings allows for more general localization regimes (e.g., on hybrid, molecular states). Systems as diverse as Mott insulators and covalent semiconductors can be described within the same theoretical framework. Also, phenomena like electron-transfer reactions or formation and breaking of bonds, whose modeling within “standard” (e.g., LDA or GGA) approximations to DFT or with the “on-site” DFT+U approach is problematic, will be addressed with higher precision. Accurate energetics is guaranteed by the consistent evaluation of V that can be obtained, at no additional cost, from the same linear-response approach used to calculate U [1]. The flexibility and reliability of the novel functional are demonstrated by its application to covalent (Si) and ionic (GaAs) semiconductors and to charge-transfer insulators (NiO). [1] M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005).

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S1.00214 Extended LDA+U+V approach for covalently bonded systems. VIVALDO LEIRIA CAMPO JR, Departamento de Fisica, Universidade Federal de Sao Carlos, Sao Carlos, Brazil, MATTEO COCCOCCIONI, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, USA — A novel DFT+U energy functional (named DFT+-U-V) is introduced based on a corrective Hubbard Hamiltonian that includes both on-site (U) and inter-site (V) electron-electron interactions. The competition between these couplings allows for more general localization regimes (e.g., on hybrid, molecular states). Systems as diverse as Mott insulators and covalent semiconductors can be described within the same theoretical framework. Also, phenomena like electron-transfer reactions or formation and breaking of bonds, whose modeling within “standard” (e.g., LDA or GGA) approximations to DFT or with the “on-site” DFT+U approach is problematic, will be addressed with higher precision. Accurate energetics is guaranteed by the consistent evaluation of V that can be obtained, at no additional cost, from the same linear-response approach used to calculate U [1]. The flexibility and reliability of the novel functional are demonstrated by its application to covalent (Si) and ionic (GaAs) semiconductors and to charge-transfer insulators (NiO). [1] M. Cococcioni and S. de Gironcoli, Phys. Rev. B 71, 035105 (2005).

S1.00215 Physical Properties of Various Materials Relevant to Granular Flow. KURT ROSENTRATER, USDA-Agricultural Research Service — Because of the ubiquitous nature of granular materials, ranging from natural avalanches to industrial storage and processing operations, interest in quantifying and predicting the dynamics of granular flow continues to increase. The objective of this study was to investigate various physical properties of common biological bulk solids (i.e., grains) which are relevant to granular flow. Particle size, shape, loose bulk density, compacted bulk density, angle of repose, and angle of marginal stability will be presented and discussed. Flow properties depend, in large measure, upon the size and shape of the particles themselves; thus information generated from this study may be useful to future experimental and simulation studies of bulk flow.

S1.00216 Bismuth nanowire array fabrication and measurements. RICHARD GRECO, Los Alamos National Laboratory — Bismuth Nanowire Arrays (BNAs) are semiconducting materials that can potentially lead to radiation detectors with better spectral resolution and efficiency than cooled high purity germanium because of the high atomic number of bismuth and expected nanowire electronic properties. Bismuth, which is normally a semi-metal, becomes a semiconductor when it is fabricated in wire form with a diameter smaller than 50 nanometers (nm). Arrays of bismuth nanowires are produced by vapor deposition into electrochemically-fabricated alumina templates. The electronic bandgap of a bismuth wire is a function of its diameter, varying from 0 eV at 50 nm to 0.7 eV at 5 nm. In this paper we present an improved fabrication technique and recent measurements on BNAs.

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S1.00217 Organic non-volatile memories from ferroelectric phase separated blends, KAMAL ASADI, University of Groningen, DAGO DE LEEUW, Philips Research Labs, The Netherlands, BERT DE BOER, PAUL BLOM, University of Groningen — Ferroelectric polarisation is an attractive physical property for non-volatile binary switching. The functionality of the targeted memory should be based on resistive switching. Conductivity and ferroelectricity however cannot be tuned independently. The challenge is to develop a storage medium in which the favourable properties of ferroelectrics such as bistability and non-volatility can be combined with the beneficial properties provided by semiconductors such as conductivity and rectification. In this contribution we present an integrated solution by blending semiconducting and ferroelectric polymers into phase separated networks. The polarisation field of the ferroelectric modulates the injection barrier at the semiconductor–metal contact. This combination allows for solution-processed non-volatile memory arrays with a simple cross-bar architecture that can be read-out non-destructively. Based on this general concept a non-volatile, reversible switchable Schottky diode with relatively fast programming time of shorter than 100 microseconds, long information retention time of longer than 10days, and high programming cycle endurance without destructive read-out is demonstrated.

S1.00218 Manganese doping of group IV semiconductor surfaces and nanostructures1, PETRA REINKE, CHRISTOPHER NOLPH, KIRIL SIMOV, University of Virginia — The combination of Si and Ge with Mn is a critical step in the development of novel spintronics devices. We investigate the magnetic doping of Si, Si-surfaces and Ge-quantum dots with Mn. A surface-driven route is used for the addition of Mn and allows a stringent control of the Mn-Si and Mn-Ge interaction. The evolution of nanostructures is observed with STM and PES. Monatomic Mn-wires form on the Si(100) surface in the low-mobility regime and dissolve into sub-surface structures at elevated temperatures. The phase diagram for Mn-Si nanostructures is developed and leads to embedded Mn structures. The interaction of Mn with Ge-quantum dots poses a new set of constraints. The Mn-addition leads to the formation of surface clusters on the wetting layer whose spatial distribution is driven by the surface relaxation. The Mn-adatom clusters on the 105 facet of the Ge-quantum dots are oriented with respect to the surface reconstruction, which predetermines diffusion pathways into the Ge-QD. The characteristics of Mn-nanostructure formation and the possibility of the synthesiss of magnetic structures will be discussed.

1Support by NSF, CTRF-Virginia, DOE-ALS is gratefully acknowledged.

S1.00219 The impact of the market index on the topology of financial networks, EDWARD MANDERE, HAO WEN XI, Bowling Green State University — We study the financial network generated from stock price returns correlation. The network topology has been used to explore and visualize the relationships between stocks. These networks have also been used in reconstructing less noisy correlation matrices for portfolio optimization. In this work, we explore the effect of adding the market index to the rest of stock network. We show that there is a very strong clustering around the index, both in S&P500 and DJIA. The mechanism that leads to these strong clustering as well as the implication to reconstructed correlation matrices will be explored.

S1.00220 Second harmonic generation in N@C60 and P@C601, MEGAN MORRIS, NICOLE PERIGO, GUOPING ZHANG, Department of Chemistry and Physics, Indiana State University, Terre Haute, IN 47809 — The successful implantation of nitrogen and phosphorus into C60 opens many new applications. For instance, both N@C60 and P@C60 are ideal candidates for quantum computing. In this paper, we show that N@C60 and P@C60 can be used to generate the second harmonic generation. If N and P are at the center of the buckyball, the signal is zero, but if they are off the center, the signal comes out. Therefore, the oscillation of N and P atoms will generate a 0-1-0-1 bit, when detected along the incident light direction. If this signal is sent to another N@C60 and P@C60, they can control the sequence of bits. The intensity sensitively depends on the laser energy and polarization. This process can be useful for quantum control by N@C60 and P@C60 themselves. All the results are obtained using the first-principles method.

1This work is supported by DOE under Contract No. DE-FG02-06ER46304, Promising Scholars grant, NERSC at LBNL under Contract No. DE-AC02-05CH11231, and Department of Chemistry and Physics, Indiana State University.

S1.00221 Quantum correlated light pulses from sequential superradiance of a condensate1, MEHMET EMRE TASGIN, MEHMET OZGUR OKTEL, Department of Physics, Bilkent University, 06800 Bilkent, Ankara, Turkey, LI YOU, School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA, OZGUR ESAT MUSTECAPLIOGLU, Department of Physics, Koc University, 34450 Sariyer, Istanbul, Turkey — We discover an inherent mechanism for entanglement swap associated with sequential superradiance from an atomic condensate. As a result, Einstein-Podolsky-Rosen (EPR)-type quantum correlated photons can be detected among the scattered light pulses.

1TUBITAK, TUBA, US NFS

S1.00222 Doping effects on charge density wave state in o-TaS2, DAMIR DOMINKO, DAMIR STARESNIĆ, KATICA BILJAKOVIC, Institute of Physics, Zagreb, Croatia, PETER LUNKENHEIMER, ALOIS LOIDL, Experimental Physik V, Augsburg, Germany, JEAN CLAUDE LASJAUNIAS, Institut Neel, Grenoble, France — We present the effects of the isoelectronic supstitution of Ta by (0.2 and 0.5 %) Nb atoms on the charge density wave (CDW) properties in o-TaS2. CLAUDE LASJAUNIAS, Institut Neel, Grenoble, France — We present the effects of the isoelectronic supstitution of Ta by (0.2 and 0.5 %) Nb atoms on the charge density wave (CDW) properties in o-TaS2. We investigate the magnetic doping of o-TaS2, and low energy excitation contribution to specific heat (Cv). The characteristic, primary relaxation process which gives the maximum in the dielectric constant near 100 K disappears with slight doping. At the same time the minimum in threshold field in the same temperature range disappears as well, which is expected from well known relation between E2 and low frequency dielectric constant [1]. This implies that the primary process it mainly due to polarization on order of domain scale, which decreases by doping. The secondary process, on the other hand, as well as low energy excitation contribution to specific heat (Cv), seem to be unchanged. Only the amplitudes of the two are increased [1, 2], as both are due to the local excitations of the CDW phase in vicinity of defects described by two level system (TLS) model. [1] Staresnii et. al, Phys. Rev. B, 65, 165109 (2002) [2] Biljakovic et. al, Europhys. Lett., 62 (4), pp. 554–560 (2003)

S1.00223 Nature of Light, SUNIL THAKUR, Independent Research — How do we perceive light? We assume that we have to absorb a photon to perceive light. When we set out to confirm this assumption experimentally then we find that everything we knew about light is wrong. We can perceive light wherever it is, provided light is in the perceivable range of our eyes. More than one photon detector can simultaneously detect a single photon. Obviously, a single photon cannot be absorbed by more than one detector. We can see a laser beam refract as it enters water from air but we find no refraction when we view the laser beam from the side of the container. It is possible only if we can see the light without having to absorb the light. Perception of the total solar eclipse as it occurs confirms this observation. All light sources emit only energy, light is produced by the object that absorbs this energy. Only difference between a luminous object and an illuminated object is that luminous objects generate their own energy to radiate light whereas illuminated objects need energy from an external source to radiate light. The observations are conclusively validated in several other advanced experiments. These observations also show that the idea of motion cannot be associated with the light; illusion of motion of light is created due to movement of energy through the medium that produces light. These experiments conclusively invalidate theory of relativity, standard model of cosmology, and standard model of particle physics.
S1.00224 Phonon Spectroscopy by Electrical Measurement in Coupled Quantum Dots. AKIKO UEDA, Department of Physics, Keio University, MIKIETO ETÓ, Faculty of Science and Technology, Keio University — We propose a phonon spectroscopy by electrical measurement in coupled quantum dots. We consider T-shaped double quantum dots, in which one of the dots is connected to external leads (dot 1) and the other is disconnected (dot 2). The differential conductance shows a dip at the midpoint of the two peaks by resonant tunneling through bonding or antibonding orbitals between the two dots, when the energy levels are tuned in the dots. The dip is caused by the destructive interference between the electron waves passing by the molecular orbitals. We calculate differential conductance under finite bias $V_{bias}$ using Keldysh Green function method. The conductance dip is diminished by electron-phonon interaction since phonon emission from dot 2 destroys the interference between electron waves passing through only dot 1 and waves passing through both dots. The dip as a function of $V_{bias}$ reflects a product of the density of states for phonons at $eV_{bias}$ and strength of electron-phonon coupling in dot 2. This implies a new method of electrically detected phonon spectroscopy.

S1.00225 Transport Properties for Biphenyl-Based Molecular Junction System. HISASHI KONDO, Institute of Industrial Science, University of Tokyo, JUN NARA, TAKAHISA OHNO, Computational Materials Science Center, National Institute for Materials Science — In the present study, the transport properties of a biphenyl-based molecule $[X\rightarrow BP\rightarrow X$: the end-group atom], $X=O$, $S$, $Se$, and $Te$ sandwiched between Au(111) electrodes are theoretically investigated using the non-equilibrium Green’s function method based on the density functional theory. The end-group atom $X$ has an influence on the interaction between the molecule and electrodes and the interaction between the two phenyl rings. For $X=O$, $S$, $Se$, and $Te$, similar transport properties are obtained, while the system with $X=O$ exhibits much different properties from the other $X$s. In case of $X=O$, the interaction between the molecule and electrodes becomes the weakest and that between $\pi$-type orbitals of the two phenyl rings, which mainly contributes to the transmission across the Fermi energy, becomes the strongest. As a result, this system has a larger transmission around the Fermi energy. We also investigate the dependence on dihedral angle between the two phenyl rings for all $X$s. This study was supported by the RISS project and a Grant-in-Aid for Scientific Research (No.17064017) of MEXT of the Japanese Government. The present calculations were performed by using the Numerical Materials Simulator in National Institute for Materials Science.

S1.00226 Electronic structure and Fermi surface of Pr$_{M}$In$_{5}$ ($M=$Co, Rh, and Ir) compounds$^1$. SAAD ELGAZZAR, Uppsala University, INGO OPAHLE, MANUEL RICHTER, PETER OPPENEER — We report density functional calculations of the electronic structure, Fermi surface, and de Haas-van Alphen (dHvA) quantities of the Pr$_{M}$In$_{5}$ ($M=$Co, Rh, and Ir) compounds. Our investigation is carried out within the framework of the local density approximation (LDA), using a relativistic, full-potential band structure method (FPLO). A critical analysis of the electronic structures and the de Haas-van Alphen quantities is performed, which shows that good agreement with recent measurements is obtained when we assume the Pr 4$f$ states to be localized. The topology of the Fermi surface is calculated to be similar to that of non-4$f$ reference compounds, as, e.g., LaRhIn$_{5}$. The similarities of the Fermi surfaces and the dHvA extremal orbits among the compounds in the series are discussed. We furthermore compare our calculated effective masses with experimental measurements and discuss the differences between them.

$^1$This work was supported by Menoufia Univ. (Egypt), the Swedish VR and SNIC and by the Deutsche Forschungsgemeinschaft, SFB 463/B11.

S1.00227 Capillary interactions in nano-particles suspensions$^1$. DOBRIN BOSEEV, GARFIELD WARREN, Indiana University — We have investigated the structures formed by colloidal particles suspended in solvents at volume fractions below 10% and interacting through capillary bridges. Such systems resemble colloidal gas of sticky nano-spheres that form pearl-necklace like chains that, in turn, induce strong viscoelasticity due to the formation of 3-D fractal network. The capillary force dominates the electrostatic and Van der Waals forces in solutions and can bridge multiple particles depending on the volume of the capillary bridge. We have investigated the morphology of the structures formed at different fractions of the bridging fluid. Computer simulations of a pearl necklace-like chain of spheres is conducted to explain the structure factor when capillary bridges are present. Alternatively, we have analyzed the slope of the neutron scattering intensity at low Q in a double logarithmic plot to determine the dimension of the fractal structures formed by the particles at different volume fraction of the bridging fluid. We have also studied the properties of the capillary bridge between a pair of particles. The significance of this study is to explore the possibility of using capillary force as a tool to engineer new colloidal structures and materials in solutions and to optimize their viscoelastic properties.

$^1$Supported by IU FRSP grant

S1.00228 Capillary interactions between silica-particles in organic solvents$^1$. GARFIELD WARREN, DOBRIN BOSEEV, Indiana University — Small-angle neutron scattering (SANS) is used to study the interactions of silica nano-particles with an average diameter of 10 nm in methanol and methanol/toluene mixtures at 25 °C. SANS intensities are analyzed as a product of a form factor and a structure factor. The form factor is experimentally determined in methanol after addition of simple electrolyte at a concentration of 100 mM to suppress the interparticle interactions. The data is successfully fitted by Hayter-Penfold mean spherical approximation (HPMSA) that yielded the specific area of surface charge in methanol. The phase behavior, viscosity and interparticle interactions are studied as a function of fraction of toluene in methanol/toluene mixtures at a constant particle volume fraction of 3.7 %. At intermediate fractions of toluene, between 44 and 65 %, the viscosity increases by two orders of magnitude which suggests formation of a new phase behavior. We will present the static magnetization and specific heat data for these pseudo-ternary compounds investigated in the necessary temperature range. Discussion of the change in the superconducting critical temperature $T_{c}$ will be directed toward the changes of electron number density as well as the lattice parameters with respect to pure LaPtSi.

$^1$Supported by the National Science Council of R.O.C. under grant no. NSC 96-2112-M-194-008-MY3.
S1.00230 Crystal structure and superconductivity in (La$_{1-x}$Y$_x$)NiC$_2$
, H.H. SUNG, K.J. SYU, T.F. LIAO, W.H. LEE, National Chung Cheng University — As observed in the powder X-ray diffraction and crystallographic data, the partial substitution of La with Y in (La$_{1-x}$Y$_x$)NiC$_2$ could be systematic up to the solubility limit near $x = 0.35$. The variation of room temperature lattice parameters, a, b, c and $\theta$ of these substitude compounds are consistent with what one would expect from a chemical pressure effect. Magnetic, electrical and heat capacity measurements indicate that the change in $T_c$ with $x$ is similar to the change in the lattice parameter. It is found that the $T_c$ change rate is $dT_c/dx = -7.0$ K and $dT_c/dv = 0.46$ K/a$^3$. According to the BCS theory, the stiffening of the lattice under pressure may change both the electron-phonon coupling strength $V$ and the electron density of states at the Fermi level, $N(0)$, which will lead to the change of $T_c$. Analysis of the electron density of states at Fermi level $N(0)$ from the specific heat data indicates that the effect of $N(0)$ on $T_c$ dominates in the (La$_{1-x}$Y$_x$)NiC$_2$ system.

S1.00231 Unbinding Dynamics of weakly adhered vesicle on a substrate , SUNITA CHATKAEW, MARC GEORGELIN, MARC LEONETTI — Unbinding dynamics of a vesicle adhering weakly on a substrate by hydrodynamic force is characterized in our works. Vesicle shapes on a substrate are governed by adhesion energy, gravity and curvature energy. Several regimes of unbinding dynamics are observed from inflated vesicles until the deflated ones. Water film growth between the membrane and the substrate and the reduction of contact area are monitored. In the case of inflated vesicle, the unbinding dynamics shows the growth of water film with the same contact area. After this lag time, the radius of the contact area decreases strongly following a 1/2 power law. When the vesicles are more deflated, the unbinding is then just a strong reduction of the contact area at a constant thickness of water film. Lipidic tube can be found in the case of a strongly applied hydrodynamic force on a deflated vesicle occupying a large contact area.

S1.00232 Particle-Tracking Velocimetric Investigation of Large Amplitude Oscillatory Shear of Entangled Polymer Melts , GREGORY ZARTMAN, YANGYANG WANG, SHI-QING WANG, The University of Akron — Large amplitude oscillatory shear (LAOS) experiments were carried out on a series of entangled monodisperse styrene-butadiene random copolymers (SBR). The deformation field during the measurements was monitored with a particle-tracking velocimetric technique. It was found that when the applied frequency was higher than the overall relaxation rate of the sample, the entangled melt would undergo uniform deformation at small strains, but exhibit shear banding at large strains. The inhomogeneity of the deformation field suggests that yielding through chain disentanglement cannot take place uniformly. This is the first report of shear banding in LAOS for melts and consequently rules out any speculation that shear banding could originate from concentration variation (due to shear induced phase separation) in entangled solutions.

S1.00233 Elementary charge-transfer processes in mesoscopic conductors , MIHAJLO VANEVIC, Georgia Institute of Technology, YULI NAZAROV, Delft University of Technology, The Netherlands, WOLFGANG BELZIG, Universit¨ at Konstanz, Germany — We determine charge-transfer statistics in a quantum conductor driven by a time-dependent voltage and identify the elementary transport processes. At zero temperature unidirectional and bidirectional single-charge transfers occur. The unidirectional processes involve electrons injected from the source terminal due to excess dc bias voltage. The bidirectional processes involve electron-hole pairs created by time-dependent voltage bias. This interpretation is further supported by the charge- transfer statistics in a multiterminal beam-splitter geometry in which injected electrons and holes can be partitioned into different outgoing terminals. The probabilities of elementary processes can be probed by noise measurements: the unidirectional processes set the dc noise level, while bidirectional ones give rise to the noise oscillations. Finally, the noise oscillations are observed to be strongly correlated with the driving amplitude. The decomposition of the noise into the contributions of elementary processes reveals the origin of these oscillations: the number of electron-hole pairs generated per cycle increases with increasing the amplitude. The charge- transfer statistics at finite temperature can be interpreted in terms of multiple-charge transfers with probabilities which depend on energy and temperature.

S1.00234 On the Salecker-Wigner-Peres Clock and Quantum Tunneling , LUÍZ MANZONI, Concordia College - Moorhead, JOSE LUNARDI, MARCOS CALCADA, Universidade Estadual de Ponta Grossa — We consider the Salecker-Wigner-Peres clock formalism and show that in the approach introduced by Peres it can be directly applied to quantum tunneling. Then we apply this formalism to the determination of the tunneling time of a non relativistic particle through a double barrier potential. In special, we consider the case in which the clock runs only when the particle can be found inside the region between the barriers and analyze the limit of opaque barriers in order to discuss the generalized Hartmann effect.

S1.00235 Restricted height discrete model , JIN MIN KIM, Soongsil University — We introduce a discrete growth model following the Edward- Willkinson equation with a conservative noise. The surface width $W$ can be found inside the region of tunneling time of a non relativistic particle through a double barrier potential. In special, we consider the case in which the clock runs only when the particle.

S1.00236 Growth of the Graphene Nanoribbons on the Vicinal 6H-SiC(0001) Surface , ILYOU KIM, E. CHO, Chonnam National University, C. HWANG, W. KIM2, KRISS — Graphene nanoribbons (GNR) are currently considered as one of the most promising materials for future nanoelectronic devices due to its exceptional physical properties. We investigated the possibility of the growth of GNR on the vicinal 6H-SiC(0001) surface using Scanning Tunneling Microscopy. We observed the formation of the ribbon-like single-layer graphene with sharp edge structures at the initial stage of thermal graphitization process of the SiC(0001) surface. However, the overall long-range ordering of the steps of the bare vicinal surface was found to be lost during graphitization process, and only the local short range ordering of the steps with graphene layer patches existed on the entire surface. From the atom-resolved STM images, we clearly identified the armchair edge structure of graphene for several ribbon-like graphene nanostructures. Scanning tunneling spectroscopy experiment was also carried out over the ribbon-like graphene patches to examine the local electronic states at the edge structures.

S1.00237 First Principles Study of Nature of Binding Energies in Solid Hydrogen , HARI PAUDEL, University of Central Florida, SITARAM BYAHUT, Tribhuvan University, Kirtipur Kathmandu, Nepal — The study of solid hydrogen is of utmost importance since it can be used as renewable source of energy. In the present work, we have quantitatively studied the properties of solid molecular hydrogen. The Hartree-Fock method, together with electron correlation effects included by many-body perturbation theory, has been utilized in this work. Study of geometry and binding energy using different basis sets will be presented. In addition to this, the effect on energy due to orientations of hydrogen molecule at lattice point will be presented and compared with available experimental data. A comparison of binding energy using pair energy approximation and cluster energy approximation methods will be discussed.

1Supported by the National Science Council of R.O.C. under grant no. NSC 96-2112-M-194-008-MY3.

2corresponding author
S.100238 Elastic yielding after step shear and shear banding in LAOS: Is there any edge effect?

XIN LI, SHI-QING WANG, The University of Akron — One of the most striking findings in our recent exploration of nonlinear rheological behavior of entangled polymers is the discovery that a suddenly sheared sample cannot relax quiescently. In both solutions \([1]\) and melts \([2]\), particle-tracking velocimetric (PTV) observations reveal macroscopic motions after a large step shear. The present work takes a significant step forward to examine whether such cohesive failure upon shear cessation could arise from the experimental imperfection due to the presence of the free surface, i.e., the meniscus. By adopting a new setup to insure that the edge only undergoes a small strain and therefore suffers no failure of any kind, we determine how the sample interior would undergo elastic yielding in the form of macroscopic motions during stress relaxation upon a large step strain. The same device also allows us to illustrate that the previously observed shear banding in large amplitude oscillatory shear (LAOS) \([3]\) is also an inherent response to the imposed LAOS, free of any edge effects. \([1]\) S. Ravindranath and S. Q. Wang, Macromolecules 40, 8031 (2007). \([2]\) P. Boukany and S. Q. Wang, Macromolecules, to be submitted (2009). \([3]\) S. Ravindranath and S. Q. Wang. J. Rheol. 52, 341 (2008).

S.100239 Exploring origins of nonlinearity in large amplitude oscillatory shear of different viscoelastic materials

XIN LI, The University of Akron, XIAORONG WANG, Bridgestone Americas Center for Research and Technology, SHI-QING WANG, The University of Akron — The present work studies nonlinear behavior in large amplitude oscillatory shear (LAOS) of three different polymeric materials using both rheometric and particle-tracking velocimetric measurements. We show that nonlinearity in LAOS is often not inherent response of the polymers that are capable of rearranging their microstructures over time. For instance, a highly viscoelastic material made of nano-sized polybutadiene particles exhibits homogeneous deformation and a nearly perfect single-harmonic sinusoidal wave in its stress response despite strong strain softening. In a second example of a well entangled polymer solution, the structural alternation in LAOS occurs non-homogeneously, where the nonlinearity also took a finite time to develop to its fullest. In the last example of wall slip, contrary to the literature claim that it should violate the mirror symmetry, the stress response only involves odd-harmonics, i.e., there is equivalence during steady-state wall slip in LAOS when the direction of shear is reversed.

S.100240 Undulatory swimming of a sandfish lizard in granular media\(^1\), DANIEL GOLDMAN, RYAN MALADEN, CHEN LI, YANG DING, Georgia Tech — We study the locomotion of the desert dwelling sandfish lizard (Scincus scincus) as it dives into and swims beneath the surface of sand (300\(\mu\)m glass beads). Above the surface, the animal uses a diagonal gait to move rapidly across the sand. High speed \(x\)-ray imaging reveals that once subsurface the animal no longer uses limbs for propulsion but instead folds the limbs against the body and generates thrust using a large amplitude undulatory motion consisting of a traveling wave with frequency \(f\) that propagates down the body with one wave period. The forward swimming speed \(v\) (maximum 10 cm/sec) increases with increasing \(f\). We measure \(v\) versus \(f\) as a function of packing fraction of the material \(\phi\). To predict \(v\) as a function of \(f\) and \(\phi\), we model the animal as a series of elements, each which produces thrust and experiences drag along its surface. We measure thrust and drag coefficients by performing drag measurements on a small stainless steel rod (grain-rod friction comparable to the animal’s skin) as a function of rod angle, rod speed, and \(\phi\). Integrating the drag law over a sinusoidal wave form accurately predicts the \(v = f\) relationship of the animal in loose and close packed granular media.

\(^1\)work supported by the NSF Physics of Living Systems

S.100241 Characteristics of top-gate ZnO thin film transistors grown on glass substrate by pulsed laser deposition, TOSHIHIKO MAEMOTO, KENJI FUJWARA, TAICHI YOSHIDA, SHIGEHKO SASA, MASATAKA INOUE, Osaka Institute of Technology — We report on the fabrication and characterization of top-gate ZnO thin film transistors (TFTs) using glass substrates. High quality ZnO epitaxial films were grown on glass substrates (Corning \#1737) by pulsed laser deposition. The thickness of the films was in the range of 50-100 nm. The growth temperature was set to 380°C. These films were characterized by \(x\)-ray diffraction, and Hall effects measurements. Highly \(c\)-axis oriented ZnO(0002) reflections corresponding to the wurtzite-phase were observed for all the films, indicating that these films grow epitaxially as a crystalline single phase on a glass substrate. The Hall effects measurements show that we have succeeded in fabricating a ZnO film with an electron mobility of 36 cm²/Vs on a glass substrate. Top-gate ZnO TFTs were fabricated by photolithography and wet chemical etching. The ohmic contact metal Ti/Au was deposited by electron beam evaporation. The top gate electrodes and the gate insulator SiO₂ were finally deposited by electron beam deposition. A room temperature characteristic of ZnO TFT with 50 \(\mu\)m gate length was an n-channel depletion type with a transconductance of 5.4 mS/mm. The off current was less than 10\(^{-9}\) A and the on/off current ratio was about 10\(^5\) at \(V_{DS} = 5\) V.

S.100242 Stabilization of Ti-Zr-Ni quasicrystals by hydrogen and application as renewable energy storage materials\(^1\), SANG-HWA LEE, JAE-KYUN JEON, SOO-BIN CHOI, JAE-YONG KIM, Hanyang University, INST TEAM — We prepared quasicrystal samples by rapidly quenching of Ti₆₃₋ₓZrₓTaₓNi₂₀ alloys (where 0 ≤ x ≤ 10), and measured equilibrium vapor pressures of hydrogen using a lab-built computer-controlled-absorption apparatus at elevated temperatures. To activate the hydrogen absorption, we removed a thin oxygen layer on the surface of the sample by using a plasma etching in a partial pressure of Ar and applied an immediate thin Pd coating by using a physical vapor deposition. As a result, the equilibrium vapor pressures of hydrogen in the QCs were lower than 5 Torr at below 300°C, and were increased as lowering the temperature. The maximum value of the H/M was also increased as increasing the temperature. Interestingly, the coherence length of the QCs was increased from 180 to 270 µm gate length was an n-channel depletion type with a transconductance of 5.4 mS/mm. The off current was less than 10\(^{-9}\) A and the on/off current ratio was about 10\(^5\) at \(V_{DS} = 5\) V.

\(^1\)This work was supported by the Korea Research Foundation Grant (KRF-2007-331-C00107) funded by the Korean Government (MOEHRD)

S.100243 Semiconductor-metal transition of Se in Ru-Se Catalyst Nanoparticles, P.K. BABU, Department of Physics, Western Illinois University, ADAM LEWERA, Department of Chemistry, Warsaw University, Poland, ERIC OLDFIELD, ANDRZEJ WIECKOWSKI, Department of Chemistry, University of Illinois at Urbana-Champaign — Ru-Se composite nanoparticles are promising catalysts for the oxygen reduction reaction (ORR) in fuel cells. Though the role of Se in enhancing the chemical stability of Ru nanoparticles is well established, the microscopic nature of Ru-Se interaction was not clearly understood. We carried out a combined investigation of \(^{125}\)Se NMR and XPS on Ru-Se nanoparticles and our results indicate that Se, a semiconductor in elemental form, becomes metallic when interacting with Ru. \(^{125}\)Se spin-lattice relaxation rates are found to be proportional to \(T\), the well-known Korringa behavior characteristic of metals. The NMR results are supported by the XPS binding energy shifts which suggest that a possible Ru—Se charge transfer could be responsible for the semiconductor→metal transition of Se which also makes Ru less susceptible to oxidation during ORR.
S1.00244 Morphology Characterization of Polymer Nanocomposites using Electron Tomography and Analytical TEM, LAWRENCE DRUMMY, UES Inc., RICHARD VAIA, Air Force Research Laboratory — Polymer nanocomposites often display complex hierarchical structures that require high resolution morphological and chemical analysis. Here we describe methods for and quantitative results from electron tomography of polymer layered silicate nanocomposites. High angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and subsequent tomographic reconstruction produced fully segmented 3D data sets from the nanocomposites. A 3D power spectrum of the fast Fourier transform (FFT) was calculated, radially integrated, and compared with the one dimensional SAXS from the same sample. As a tool for determination of nanoparticle global dispersion, the analysis revealed good agreement between the techniques from the sub-nm regime up to a length scale of 1 micron. Currently, energy filtered TEM and energy dispersive spectroscopy in STEM mode are being investigated for providing high spatial resolution chemical information at interfaces and inhomogeneities in polymer nanocomposites.

S1.00245 Interlayer Thermal Coupling of Hot Dirac Fermions in Epitaxial Graphene, DONG SUN, CHARLES DIVIN, TEO NORRIS, CLAIRE BERGER, WALT DE HEER, PHILLIP FIRST, CENTER FOR ULTRAFAST OPTICAL SCIENCE, UNIVERSITY OF MICHIGAN, ANN ARBOR, MI 48109-2099 COLLABORATION, DEPARTMENT OF PHYSICS, GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA, GA, 30332 COLLABORATION — Degenerate and nondegenerate ultrafast pump-probe spectroscopy is used to study interlayer thermal coupling of hot Dirac Fermions in carbon face epitaxial graphene. The hot carriers in lightly doped and undoped graphene layers are selectively excited by the pump laser while leaving the carriers in the heavily doped layer not directly excited. Within the 500fs, carriers at elevated temperature in the heavily doped layer is observed, which is excited due to the interlayer thermal coupling of the hot carriers.

S1.00246 Exploring origin of instabilities in pressure-driven flow of entangled polymers using particle-tracking velocimetric method, XIANGYANG ZHU, SHI-QING WANG, University of Akron — Well entangled polymeric materials undergo extrudate distortions commonly known as sharkskin (semifluid melt state) and gross melt fracture. Particle-tracking velocimetric (PTV) observations have been carried out to explore the relationship between gross melt fracture and entry flow instability based on polybutadiene melts. The sharkskin formation process has also been investigated based on PTV visualization of the flow field at the die exit. These instabilities have been studied in terms of the material parameters.

S1.00247 Morphology and structure of the self assembled Ag nanodots on undoped Si(100) under ambient conditions, JEFFREY PARKS, INDIRAJITH SENEVIRATHNE, Lock Haven University of Pennsylvania — Self assembly is an important bottom up design approach in making nanostructures on substrate. Therefore understanding the self assembly mechanisms is very important. Morphology and structure of the self assembled Ag nano dots via sputter deposition on the chemically cleaned ambient undoped Si(100) wafer at RT (−300K) is observed via contact mode Atomic Force Microscopy (AFM). At a Ag coverage of ∼60ML nucleation of the nanodots were seen, implying StranskiKratov growth mode. At a coverage of ∼120ML the self assembled nanodots are clearly seen. These nanodots are observed to have ∼40nm in width and ∼10nm in height. At increase Ag coverage (∼120ML and ∼180ML) it is observed the number density of Ag nanodots increase in lock step. Higher the coverage size characteristics observed to show a higher variance. When annealed at successively higher temperatures (∼373K, ∼473K, ∼573K) for an interval of 5min the structures seem to dissolve, implying kinetically limited growth. Conductivity measurements on these nanostructures will also be discussed.

S1.00248 Study on the formation of rhenium borides by density functional calculations, R.R. AGUNDEZ, Facultad de Ciencias, UABC, G. SOTO, M.G. MORENO, A. REYES-SERRATO, Centro de Nanociencias y Nanotecnologa, UNAM — The searching of hard and superhard materials is a hot topic in material science. Two known factors are fundamental to get high hardnes: (1) high valence-electron density; and (2) high number of electron in covalent bonds. The 5d-transition metals comply with requirement (1); so, the task is to fulfill condition (2) without expanding its native structure. Supposedly this is possible by developing interstitial alloys with elements of moderate electronegativity, like boron and/or carbon. This idea materializes in the very hard ReB2, which scratches the surface of diamond. This work is a study in the formation of rhenium borides by density functional calculations. Here, we want to reveal the changes that would occur in the hexagonal close packed lattice of Re as B is inserted into its interstitial sites. We cover compositions in ReBx from x = 0 to x = 3 in x steps of 0.125. B is positioned in octahedral and tetrahedral interstices of Re, and for each arrangements we have calculated cell volume, cohesive energy, bulk modulus, valence electron concentration, and energy density. Supported by FONDOS CONACyT 10013, SNI-ESTUDIANTES 2008-01, SOLICITUD: 103909.

S1.00249 Magnetic force microscopy studies of vortex states in type II superconductors and ferrromagnetic microstructures, JEFFREY WRIGHT, UCLA Department of Physics and Astronomy, EVGUENI NAZARETSKI, Los Alamos National Laboratory, P. C. HAMMLE, Ohio State University Department of Physics, ROMAN M.ovshovich, Los Alamos National Laboratory — A variable temperature, high sensitivity Magnetic Force Microscope (MFM) was used to study vortices in a superconducting niobium thin film, as well as ferromagnetic microstructures, whose magnetization forms a vortex ground state. The highly sensitive interferometric detection of the cantilever displacement allowed for detailed measurements of the magnetic field profile produced by individual vortices. The MFM’s variable temperature ability and superconducting magnet allowed for field cooling of the niobium sample in an external magnetic field either parallel or anti-parallel to the orientation of the cantilever magnetic tip. MFM studies of 50 nm thick and 4 μm diameter permalloy microstructures were performed at room temperature and at 4.2K. At room temperature, the sample’s magnetization exhibited the dipole structure while at 4.2K it showed the evidence for a higher variance. By merging the MFM tip close to the sample we were able to reverse the orientation of individual vortices.

S1.00250 Simulation Coherent Quantum Processes in Many-Body Systems Using Classical Trajectories, CRAIG MARTENS, University of California, Irvine — We describe a method for the simulation of coherent quantum dynamics in many-body systems. The approach is based on the semiclassical limit of the multistate quantum Liouville equation and solution using classical trajectory ensembles. The method is applied to modeling nonadiabatic quantum dynamics and the creation, evolution, and decay of quantum coherence in condensed phase systems. The role of environmental interactions in inducing—or delaying—ultrafast electronic decoherence of molecules in condensed phases is investigated. In addition, simulations of vibrational dephasing of an I2 diatomic molecule in cryogenic rare gas matrices are described. For I2 in Kr, excellent agreement with recent experimental results is obtained.

S1.00251 Effect of Atmospheric Conditions on Type and Depth of Polymer Damage Due to Ultra Violet Radiation, MACKENZIE SINDEN-REDDING, FROUZEH SABRI, J. COLE, University of Memphis, N. LEVENTIS, Missouri Science and Technology — The Earth’s atmosphere scatters, absorbs, and reflects the sun’s total incoming radiation reducing it by nearly 55%, thus also reducing UV which causes material damage at the Earth’s surface. Visually noticeable material changes often associated with UV exposure is a color shift, typically towards a yellow tint. In this work, we have explored the relationship between free radical generation and the color shift of two types of material: RTV 655 and Silica aerogels. The impact of atmospheric conditions on the amount and nature of free radicals generated, as well as the color shift, is the prime focus of this work. Both materials are of particular interest in space-related applications such as calibration targets for Mars landers. Investigative tools implemented are ESR technique, UV-Vis spectral analysis and X-ray diffraction studies. Both material types demonstrate a significant and similar spectral shift regardless of the presence or absence of atmospheric oxygen. However, not both exposure circumstances lead to a detectable ESR signal.
Surface layer. Regardless of surface morphology, the film-bulk is electronically and magnetically active. Many of the reported conclusions about electronic phase separation; rough films are phase separated while atomically flat films are homogeneous but have a more or less inactive structural distortions.

Ultrafast dynamics of plasma microclouds induced by strong-field ionization in atomic and molecular gases. Ryan Compton, Alex Filin, Dmitri Romanov, Robert Levits, Department of Physics, and Center for Advanced Photonics, Temple University, Philadelphia PA 19122 — The model presented for the ultrafast dynamics of laser-induced plasma channels reveals the connections among the fundamental processes of laser-induced tunnel ionization, plasma cooling dynamics of the produced plasma channel, and the residual fluorescence of the channel. The results obtained link the dynamic behavior of the underdense plasma formation with the internal degrees of freedom of the constituent species suggesting that related processes of much current interest, such as laser induced breakdown, laser induced ablation, and, further, atmospheric filamentation will depend sensitively on atomic and molecular constituents. This opens the way to optimizing plasma channel characteristics (bandwidth, coherence, brightness) to that desired for a particular experiment.

Attosecond dynamics of strong-field multielectron excitation in small molecules: the case of carbon dioxide. Stanley Smith, Dmitri Romanov, Temple University, Xiaosong Li, University of Washington, H. Bernhard Schlegel, Wayne State University, Robert Levits, Temple University — The electron dynamics of CO₂ interacting with a short IR (1.63 eV) three cycle pulse was theoretically investigated, as manifested by the instantaneous dipole oscillations. The pulse envelope shape (Gaussian or trapezoidal) is shown to control the residual dipole oscillations spectrum (which excited states are populated) and amplitude (or relative population in each state). The carrier envelope phase (for either envelope shape) changes markedly the excited state amplitudes. The windowed Fourier transform was used to extract the attosecond electron excitation dynamics during the pulse. This analysis shows the nonlinear excitation process to be much more complicated than the traditional excited state ladder climbing. In particular, (i) electron transfer plays a major role in the nonlinear excitation dynamics, and (ii) the two pronounced spectral peaks at ∼5 and ∼8.5 eV do not correspond to any single-phonon dipole-allowed transitions. The electron response in the directions orthogonal to the molecular axis was also simulated and, as expected, this response was smaller in magnitude than the response along the molecular axis.

Doping the golden buckyball: M@Au₁₆ clusters. Lei-Ming Wang, Wei Huang, Lai-Sheng Wang, Xiaocheng Zeng Collaboration, Detlef Schöoss Collaboration — The 16-atom gold cluster (Au₁₆) was previously found to possess an unprecedentedly hollow cage structure. Using photoelectron spectroscopy and density functional theory, we have investigated the possibility of doping the Au₁₆ cage with an external atom, M@Au₁₆ (M = Cu, Ag, Zn, In, Si, Ge, Sn, Fe, Co, Ni). We have found that doping the Au₁₆ cluster with a Cu, Ag, Zn or In atom does not significantly alter its structure, and the dopant atom sits inside with little distortion to the parent cage. However, the Si, Ge, Sn, atoms cannot be doped inside the Au₁₆ cage and they are found to completely change the structure of the parent cage due to the strong M-Au local interactions. The transition-metal-atom-doped species, M@Au₁₆ (M = Fe, Co, Ni), are found to be endohedral in nature with atomic-like magnetic moments and some minor structural distortions.

Correlations Between Thin-Film Manganite Morphology, Phase Separation, and Dead Surface Layers Investigated with STM. Simon Kelly, Federica Galli, Ivan Komissarov, Jan Aarts, Univ of Leiden — Thin-film colossal magnetoresistance manganites such as La₁₋ₓCaₓMnO₃ have now been intensively studied for more than a decade, but the issue of possible nanoscale electronic phase separation remains unresolved. Scanning Tunneling Microscopy / Spectroscopy (STS) has been pivotal in studying phase separation, but is hindered by being surface- rather than bulk-sensitive. For our sputtered LCMO films the data indicates a strong correlation between surface morphology and phase separation; rough films are phase separated while atomically flat films are homogeneous but have a more or less inactive surface layer. Regardless of surface morphology, the film-bulk is electronically and magnetically active. Many of the reported conclusions about electronic inhomogeneities measured by STS have been confused by this issue.

Enhancement in flux pinning in superconducting Bi-Sr-Ca-Cu-O. H. Yetis, A. Kilic, K. Kilic, A. Altinkok, M. Olutas, Abant Izzet Baysal University — It is shown that the pinning properties of Bi₁₋ₓPbₓBa₂Sr₂Ca₃Cu₄O₈₋₉ (BSCO) can be increased by drilling a macroscopic cylindrical hole (CH). To observe the enhancement in flux pinning two different standard and reverse procedures in measuring of the I − V curves were performed as functions of transport current (I), temperature (T) and external magnetic field (H). For a better description, during the measurements, the sweep rate (dI/dt) of transport current in I − V curves was varied. As the current cycles in up and down direction, it was observed that the presence of CH drilled in BSCO sample causes a dramatic increase in the hysteresis effects in I − V curves depending on dI/dt and changes the evolution of I − V curves as compared to that of similar measurements carried out in BSCO sample before drilling CH. Another important observation is the increase in the critical current value of BSCO with CH for increasing branch of I − V curve. The increase in width of hysteresis loops of I − V curves was interpreted as a kind of superheated regions. We show in this study that the surface effects in superconductors can be studied by applying the reverse procedure in I − V curves. Finally, it is also shown that the macroscopic cylindrical hole act as a macroscopic pinning center for flux lines.

The new piezoelectric single crystal obtained by the Ge doping in the α-quartz structure. M. Miclau, A. Grozescu, R. Bucur, M. Poenar, P. Vlazan, I. Grozescu, Natl. Institute R&D Electrochemistry and Condensed Matter, Romania, N. Miclau, Politehnica University, Romania, I. Muscutaru, Baldwin Wallace College, USA — The most interesting properties of the quartz-like crystals are its piezoelectric properties, which are strongly influenced by the intrinsic structural distortions of the material and the crystal growth conditions. Thus, physical properties such as coupling coefficient, the α ↔ β transition can be directly related to structural distortions in terms of the bridging angle. We propose a new way to increase the structural distortion, using Ge to dope the SiO₂ structure with respect to α-quartz structure type. Growth of α-SiGe₁₋ₓO₂ crystal was realized hydrothermally using a temperature gradient method. Single crystals were investigated by electron microprobe analysis, X-ray diffraction and atomic force microscopy. The results open the possibility to tune the piezoelectric properties of these materials by varying the chemical composition.
S1.00259 Fabrication and Characterization of Si Nanorod Arrays as Subwavelength Antireflection Structures, YI-RUEI LIN, JR-HAU HE, Natl Taiwan Univ — The structure of antireflection (AR) is widely utilized to suppress undesired reflection between different optical media for various optical applications. For example, Multilayered coatings are used on the surface of optical and optoelectronic devices. However, it is also suffered from the problems such as poor adhesion, thermal instability, and lattice mismatch. An alternative to multilayered coatings is to pattern the surface with a periodically structured array with the periodicity smaller than the wavelength of the incident light. Compared with multilayered AR coatings, subwavelength structure (SWS) surfaces are more stable and durable, because the AR structures are directly etched in the surface and there are no other materials involved. So far SWSs has been fabricated on silicon have been fabricated through various methods. In the present work, we demonstrated a simple method, which combines sub-wavelength-scale monolayer spheres with a reactive ion etching process, to fabricate AR structures of Si nanorod arrays (NWAs) with structural stability, low cost, and low temperature procedures. It was found that the reflectivity of Si substrates with NWAs was dramatically decreased at the wavelength of light from 400 to 800 nm. The reflectivity as a function of size of Si NWAs was discussed.

S1.00260 Reduction of thermal conductivity on n-type silicon germanium bulk alloy with nano-pores formation, XIAOWEI WANG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, MILDRED DRESSELHAUS, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, GANG CHEN, Department of Mechanical Engineering, Massachusetts Institute of Technology, ZHIFENG REN, Department of Physics, Boston College, YUCHENG LAN, GAOHUA ZHU, GIRI JOSHI, DEZHI WANG, JIAN YANG, Department of Physics, Boston College, HOHYUN LEE, Department of Mechanical Engineering, University of Kansas, XIAOWEI WANG, Department of Physics, Boston College, HROW-MEE HO, Department of Electronic Engineering, National Taiwan University. Silicon-Germanium (SiGe) alloys have been the main thermoelectric materials in power generation devices operating from 500 °C to 1000 °C. The main challenge for enhanced thermal performance of Si-Ge system is the reduction of thermal conductivity. Here we report that by creating nano-pores, the thermal conductivity can be reduced to around 2 Wm⁻¹K⁻¹ with a little lower power factor. The nano-structured bulk alloy was made by first forming alloyed nano-pores from commercial grade Si and Ge chunks with the dopant phosphorous (P) powder and sulfur powder and then by hot pressing the powders for their compaction. Followed by annealing at 1050 °C, nano pores were created inside the bulk disc. Our results showed that nano pores are very effective to scatter phonons, thus reduce the thermal conductivity.

S1.00261 The Transition of Two Dimensional Hard Spheres Under Gravity from the Liquid to Solid State Using a Global Equation of State, ALISON E. KOSER, PAUL V. QUINN, SR., Kutztown University — Using a global equation of state, derived empirically from Liding, we can accurately model the density profile of two-dimensional hard spheres with diameter d and man cm under gravity temperature T\(_c\) and T\(_f\). When we compare our theoretical density profiles to MD simulated data, in a given system, if the temperature is below some critical value T\(_c\) obtained by the density profile, then crystallization occurs and we can solve for the number of frozen layers. Again, we compare out theoretical values for number of frozen layers with the number of frozen layers from the simulated data. In addition, we use the global equation to solve for the center of mass and its fluctuations as a function of T.

S1.00262 Geometrical Optics and Subwavelength Antireflection, CHOONG-HEE PARK, EFI, LTD., S. SHIN, RESEARCH CENTER OF MATERIALS SCIENCE, Tokyo Institute of Technology, Y. KAMIHARA, Materials and Structural Lab. Tokyo Inst. Tech., T. SHIMOJIMA, K. ISHIZAKA, T. KISS, M. OKAWA, ISSP U. Tokyo, X.-Y. WANG, C.-T. CHEN, CAS, Y. KAMIHARA, ERATO-SORST JST, in FRC, Tokyo Inst. Tech., M. HIRANO, Materials and Structural Lab. Tokyo Inst. Tech., S. SHIN, ISSP U. Tokyo — Laser photoemission spectroscopy is employed to investigate the electronic structures of LaFeAsO:F and LaFePO:F. We also find the high-T\(_c\) phase in LaFePO:F. LaFeAsO:F exhibits a temperature-dependent pseudogap extending over ~0.1 eV about the Fermi level at 250 K, whereas such a feature is absent in low-T\(_c\). LaFePO:F. We also find ~20-meV pseudogap features and signatures of superconducting gaps both in LaFeAsO:F and LaFePO:F. We discuss possible origin of the pseudogaps through comparison with the cuprates. [1] Y. Kamihara et al., JACS 128, 10012 (2006); 130, 3296 (2008). [2] Y. Ishida et al., arXiv:0805.2647.

S1.00263 Examination of the Motion of a System of Granular Material Subjected to Vertical Vibration, CARL E. FAUST, PAUL V. QUINN, SR., Kutztown University — Experiments are conducted using various granular materials subject to a vertical vibration. Qualitative data for the angle of repose is collected as a function of the initial height of the material in the container. Data is used to determine empirical relationships between the maximum angle of repose and container size. This is done for various materials of differing grain size. Also, qualitative observations are made of the surface shape and precession of the angle of repose.

S1.00264 Study of the operational properties of the Capillary Plasma Electrode (CPE) discharges, JOSE LOPEZ, DAVID JACOME, WEI-DONG ZHU, Saint Peter’s College, MARGARET FIGUS, Merck & Co., Inc., KURT H. BECKER, Polytechnic Inst. of NYU — Various approaches have been pursued to create stable atmospheric pressure discharges by extending the lifetime of the diffuse phase of the discharge to hundreds of microseconds. Previous research showed that the stability of the diffuse mode is dependent on the frequency (in the kHz range), gas type, mode of the excitation, and geometrical confinement. Some of the most promising approaches are based on the recognition of the arc formation in high-pressure plasmas can be avoided and stable high-pressure plasma can be generated and maintained when the plasma are spatially constricted to the dimensions of tens to hundreds of microns. The Capillary Plasma Electrode (CPE) discharge is stable to produce stable atmospheric pressure nonequilibrium plasma. The CPE is similar in design to the Barrier Electrode Discharge, but has perforated dielectrics. The configuration, aside from exhibiting a diffuse mode of operation, also exhibits the so-called “capillary jet” mode, in which the capillaries turn on and a bright plasma jet emerges from the capillaries. The capillary jets from adjacent capillaries overlap so that the discharge appears uniform when the electrode contains an array of holes. There appears to be a threshold frequency for the capillary jet formation, which is strongly dependent on the L/D ratio of the capillaries, where D is the diameter of the capillary and L its length. However, the operating principles and basic properties of this behavior are not well understood. The current work explores these modes of operations of the CPE by characterizing the electrical and optical emission properties of this discharge by examining a multi-hole discharge as well as a single capillary discharge reactor.

S1.00265 Direct Current Cathode Boundary Layer Xenon Discharge, WEI-DONG ZHU, LUAN TO, JOSE LOPEZ, Department of Applied Science and Technology, Saint Peter’s College, KURT BECKER, Polytechnic Inst. of NYU — Cathode boundary layer (CBL) discharge is a diffuse atmospheric pressure glow discharge usually generated between a capillary and a ring-shaped anode, separated by a dielectric layer with a thickness of several hundred micrometers. Self-organized patterns formation, excimer emission, and electrical properties of CBL discharges in a direct current operation have been thoroughly studied by Schoenbach and co-workers at various pressures in xenon with mainly molybdenum as the electrode material. However, no detailed assessment of the effect of the cathode material on the self-organized pattern formation and cathode material modification by the CBL discharge has been reported. This study focuses on the electrical characteristics of the cathode material on the cell-organized pattern formation and cathode material modification by the CBL discharge. We have investigated the effects of several cathode materials at pressures of 100 Torr and 250 Torr. Cathode material modification by CBL discharge will be briefly assessed.
3:06PM T1.00002 Ultrasensitive magnetometry and magnetic resonance imaging using cantilever detection1, DANIEL RUGAR, IBM — Micromachined cantilevers make remarkable magnetometers for nanoscale measurements of magnetic materials and for magnetic resonance imaging (MRI). We present various applications of cantilever magnetometry at low temperature using cantilevers capable of attoneutron force sensitivity. Small, unexpected magnetic effects can be seen, such as anomalous damping in magnetic field. A key application is magnetic resonance force microscopy (MRFM) of both electron and nuclear spins. In recent experiments with MRFM-based MRI imaging, 3D spatial resolution better than 10 nm was achieved for protons in individual virus particles. The achieved volumetric resolution represents an improvement of 100 million compared to the best conventional MRI. The microscope is sensitive enough to detect NMR signals from adsorbed layers of hydrocarbon contamination, hydrogen in multilayer carbon nanotubes and the phosphorus in DNA. Operating with a force noise on the order of 6 aN per root hertz with a magnetic tip that produces a field gradient in excess of 30 gauss per nanometer, the magnetic moment sensitivity is ~0.2 Bohr magnetons. The corresponding field sensitivity is ~3 nT per root hertz. To our knowledge, this combination of high field sensitivity and nanometer spatial resolution is unsurpassed by any other form of nanometer-scale magnetometry.

1Work performed in collaboration with H. J. Mamin, M. Poggio, C. L. Degen, T. Oosterkamp and C. T. Rettner

3:42PM T1.00003 Ferromagnetic Resonance Imaging with Magnetic Resonance Force Microscopy, DENIS PELEKHOV, The Ohio State University — Magnetic resonance force microscopy achieves very high resolution three-dimensional imaging capabilities of magnetic resonance imaging by taking advantage of very high sensitivity mechanical force detection. This enables non-contacting, microscopic studies and imaging of a broad range of materials. As a consequence of the strong interactions between spins, the assumptions underlying conventional MRI are not applicable to FMR imaging. However, using a new approach to localizing the resonant volume in an FMR measurement founded on the strong, nonuniform magnetic field of the micromagnetic probe tip, we have demonstrated scanned probe Ferromagnetic Resonance (FMR) imaging [1]. The scanned probe FMR images obtained in patterned ferromagnetic films are well explained by detailed numerical modeling. In addition to illuminating the mechanisms underlying localized FMR, the model provides the basis for submicron scanned probe FMR imaging of films and buried ferromagnetic elements. This work was supported by the U.S. Department of Energy through Grant No. DE-FG02-03ER46054.


4:18PM T1.00004 Ultrafast magnetization dynamics of cobalt nanoparticles and individual ferromagnetic dots, JEAN-YVES BIGOT, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR7504, CNRS-ULP, Strasbourg 67034 — The ultrafast magnetization dynamics of magnetic materials can be investigated using femtosecond laser pulses to perform femtosecond magneto-optical Kerr and Faraday measurements [1]. In this talk, we will focus on the magnetization dynamics of cobalt nanoparticles which are either ferromagnetic or super-paramagnetic at room temperature and on the dynamics of individual ferromagnetic dots. In the first case (Co nanoparticles), we will demonstrate that the magnetization dynamics preceding the fluctuations over the anisotropy energy barrier is coherent but exhibits a strongly damped precession [2]. These results, which have been obtained with a three dimensional analysis of the magnetization vector [3] will be discussed in the context of the Néel-Brown models involving the gyromagnetic character of the magnetization. We will also examine the dynamics of self-organized supra-crystals of cobalt nanoparticles [4]. In the second case, we will present the ultrafast magnetization dynamics of individual ferromagnetic dots (COPt3, Permalloy, Nickel) made either by e-beam lithography or induced optically on thin films deposited on sapphire and glass substrates. The technique employed is the magneto-optical pump probe imaging (MOPPI) which allows performing time resolved magnetic-optical Kerr images with with spatial and temporal resolutions of 300 nm and 150 fs [5]. The study of the demagnetization of the dots for different laser intensities shows that it is possible to write and read ultrafast monodomains on thin films.


4:54PM T1.00005 Magnetic soft X-ray microscopy: Towards imaging ultrafast spin dynamics on the nanoscale1, PETER FISCHER, CXRO/LBNL Berkeley CA — Modern magnetic microscopies are challenged with providing spatial resolution in the nanometer regime, a time resolution on a fs scale and elemental specificity to allow for studying multifunctional magnetic nanostructures and their ultrafast spin dynamics. Magnetic soft X-ray microscopy combines X-ray magnetic circular dichroism (X-MCD) as element specific magnetic contrast mechanism with high spatial and temporal resolution. Fresnel zone plates provide a spatial resolution down to currently <15nm [1] with current developments approaching the 10nm regime thus approaching fundamental magnetic length scales. Utilizing the inherent time structure of current synchrotron sources fast magnetization dynamics with 70ps time resolution, limited by the lengths of the electron bunches, can be performed with a stroboscopic pump-probe scheme. Soft X-ray microscopy at upcoming high brilliant fsc X-ray sources makes snapshot images of fsc spin dynamics feasible. In this talk I will present recent results on the study of the stochastic character in magnetization reversal and domain wall pinning [2] as well as on time resolved imaging of current induced resonant vortex core motion which allows to determine spin polarization of currents [3]


1This work was supported by DOE, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T1 DCMP: Probes of Nanoscale Magnetism Spirit of Pittsburgh Ballrom A

2:30PM T1.00001 Chiral magnetic order at surfaces driven by inversion asymmetry, MATTHIAS BODE, Argonne National Lab — No abstract available.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T2 DCMP DMP: Electron, Exciton and Phonon Interactions in Nanoparticles Spirit of Pittsburgh Ballrom BC
3:06PM T2.00002 Controlled Crystallinity and Fundamental Coupling Interactions in Nanocrystals

MIN OUYANG, University of Maryland at College Park — Metal and semiconductor nanocrystals show many unusual properties and functionalities, and can serve as model system to explore fundamental quantum and classical coupling interactions as well as building blocks of many practical applications. However, because of their small size, these nanoparticles typically exhibit different crystalline properties as compared with their bulk counterpart, and controlling crystallinity (and structural defects) within nanoparticles has posed significant technical challenges. In this talk, I will firstly apply silver metal nanoparticles as an example and present a novel chemical synthetic technique to achieve unprecedented crystallinity control at the nanoscale. This engineering of nanocrystallinity enables manipulation of intrinsic chemical functionalities, physical properties as well as nano-device performance [1]. For example, I will highlight that electron-phonon coupling constant can be significantly reduced by about four times and elastic modulus is increased ~40% in perfect single crystalline silver nanoparticles as compared with those in disordered twinned nanoparticles. One important application of metal nanoparticles is nanoscale sensors. I will thus demonstrate that performance of nanoparticles based molecular sensing devices can be optimized with three times improvement of figure-of-merit if perfect single crystalline nanoparticles are applied. Lastly, I will present our related studies on semiconductor nanocrystals as well as their hybrid heterostructures. These discussions should offer important implications for our understanding of the fundamental properties at nanoscale and potential applications of metal nanoparticles.


3:42PM T2.00003 New Developments in Nanocrystal Lasing: Type-II Nanostructures and “Giant” Quantum Dots

VICTOR KLIOMOV, Los Alamos National Laboratory — Nanocrystal (NC) quantum dots show high photoluminescence quantum yields and size-dependent emission colors tunable through the quantum-confinement effect. Despite their favorable light-emitting properties, NCs are difficult to use in optoelectronic applications due to a low balance between carrier absorption and stimulated emission in nanocrystals excited with single excitons. Optical gain can only occur due to NCs that contain at least two excitons. A resulting complication is fast optical-gain decay induced by nonradiative Auger recombination, a process in which one exciton recombines by transferring its energy to another. In this talk, I will discuss two approaches for resolving the problem of ultrafast Auger recombination in NCs. In one approach, we utilize core/shell hetero-NCs engineered in such a way as to spatially separate electrons and holes between the core and the shell (type-II heterostructures). The resulting imbalance between negative and positive charges produces a strong local electric field, which induces a large, ~100 meV transient Stark shift of the absorption spectrum with respect to the luminescence band. This effect breaks the exact balance between absorption and stimulated emission and allows us to demonstrate optical amplification in the single-exciton regime when Auger recombination is simply inactive. In another approach, we use recently developed “giant” dots that comprise a small emitting CdSe core overcoated with a thick shell (up to 20 monolayers) of a wider-gap CdS. These nanostructures produce a peculiar quasi-type-II localization regime, which develops as a result of a significant difference in effective volumes of the electron and hole wave functions. These structures show greatly suppressed Auger recombination, which allows us to realize broadband optical gain (extends over Δ~400 meV) due to multie excitons of various orders with an excitation threshold, which is at least a thousand times lower than in regular CdSe NCs.

4:18PM T2.00004 Plasmon-enhanced Absorption, Modulation and Spontaneous Emission in Semiconductor Quantum Dots and Films

HARRY ATWATER, California Institute of Technology — Recent advances in plasmon dispersion and localization in quantum dot layers and semiconductor thin films have enabled study of several phenomena in coupled metal/semiconductor nanophotonic structures, including i) enhanced spontaneous emission in quantum dots, ii) all-optical modulation of plasmon propagation in quantum dot active media, and iii) enhanced absorption in plasmonic solar cells. Metal-dielectric plasmon waveguides with quantum dot active layers can serve as switching elements when the complex refractive index is actively modulated. We demonstrate all-plasmonic modulation in which the complex refractive index seen by a surface plasmon polariton at an infrared free-space wavelength of 1420 nm is modulated via interband excitation of the quantum dots at a visible wavelength of 514 nm. Metallic nanostuctures can excite surface plasmons which can dramatically increase the optical path length in thin active photovoltaic layers to enhance overall photoabsorption, with potential for increased photovoltaic conversion efficiency, and new solar cell device designs. The strong mode localization of surface plasmon polaritons at metal-dielectric interfaces leads to strong absorption in very thin semiconductor films, enabling a dramatic (10-100X) reduction in the semiconductor absorber physical thickness needed to achieve optical thickness. Modal analysis in full wave simulation allows us to determine the fraction of power absorbed for both dielectric waveguide and plasmonic modes in a thin solar cell.

4:54PM T2.00005 Exciton-plasmon interactions and energy transfer in nanoparticles

ALEXANDER GOVOROV, Ohio University — Energy transfer between optically-excited nanocrystals coupled by the Coulomb interaction can be very efficient. The interaction of excitons and plasmons in nanocrystals leads to several effects: energy transfer between nanoparticles (NPs), electromagnetic enhancement, reduced exciton diffusion in nanowires (NWs), exciton energy shifts, and interference and non-linear phenomena [1-3]. Using kinetic equations for excitons, we model exciton transport in a NW and explain the origin of the blue shift of exciton emission observed in the recent experiments on hybrid NW-NP assemblies [2]. We also model artificial light-harvesting complexes composed of chlorophylls, bacterial reaction centers, and NPs [3]. Using superior optical properties of metal and semiconductor NPs, one can strongly enhance the efficiency of light harvesting [3]. An interaction between a discrete state of exciton and a continuum of plasmonic states can give rise to interference effects (Fano-like asymmetric resonances). These interference effects greatly enhance visibility of relatively weak exciton signals and can be used for spectroscopy of single nanoparticle and molecules. In the nonlinear regime, the Fano effect becomes strongly amplified [4]. In conclusion, our theory explains present experimental results and also provides motivation for future experiments and applications. Potential applications of dynamical exciton-plasmon systems include sensors and light-harvesting. The above theoretical studies were performed in collaboration with several groups [1-4].


Supported by NSF and Air Force Research Labs.
the collection of information from wideband signals such as noise, and an entry into the domain of quantum electrical signals. I will review some of our early devices are not well-matched to the fifty ohm world of microwaves, the ability to listen to signals coming from a cryogenic nanostructure with a wideband

Devices, ROBERT SCHOELKOPF, Departments of Applied Physics and Physics, Yale University — Typical measurements of mesoscopic devices at low temperatures suffer from annoyingly low speeds and the presence of excess low-frequency noise that can try the experimentalist’s patience. Even though these devices are not well-matched to the fifty ohm world of microwaves, the ability to listen to signals coming from a cryogenic nanostructure with a wideband amplifier at gigahertz frequencies has proven quite beneficial. These techniques can be surprising precise and powerful, allowing access to high-speed dynamics, the collection of information from wideband signals such as noise, and an entry into the domain of quantum electrical signals. I will review some of our early experiments at Yale in this area, especially the development of the Radio-Frequency Single-Electron Transistor (RF-SET), which is still the most sensitive electrometer known. Today we find that microwave measurements are proving highly beneficial for solid-state quantum computing, which in turn is leading to a new wave of capabilities for generating and measuring microwave signals at the single photon level.

3:06PM T3.00002 Near-Quantum-Limited SQUID Amplifier, JOHN CLARKE, University of California, Berkeley and Lawrence Berkeley National Laboratory — The SET (Single-Electron Transistor), which detects charge, is the dual of the SQUID (Superconducting QUantum Interference Device), which detects flux. In 1998, Schoelkopf and co-workers introduced the RFSET, which uses a resonance circuit to increase the frequency response to the 100-MHz range. The same year saw the introduction of the Microstrip SQUID Amplifier (MSA) in which the input coil forms a microstrip with the SQUID washer, thereby extending the operating frequency to the gigahertz range. I briefly describe the theory of SQUID amplifiers involving a tuned input circuit with resonant frequency \( f \). For an optimized SQUID at temperature \( T \), the power gain and noise temperature are approximately \( G = f / f_p \) and \( T_N = 20 \pi f f_p \), respectively, where \( f_p \) is the plasma frequency of one of the Josephson junctions. Because the SQUID voltage and current noise are correlated, however, the optimum noise temperature is at a frequency below resonance. For a phase-preserving amplifier, \( T_N = (1/2 + A)hf/k_B \), where Caves’ added noise number \( A = 1/2 \) at the quantum limit. Simulations based on the quantum Langevin equation (QLE) suggest that the SQUID amplifier should attain \( A = 1/2 \). We have measured the gain and noise of an MSA in which the resistive shunts of the junctions are coupled to cooling fins to reduce hot electron effects. The minimum value \( A = 1.1 \pm 0.2 \) occurs at a frequency below resonance. On resonance, the value \( A = 1.5 \pm 0.3 \) is close to the predictions of the QLE, suggesting that this model may fail to predict the cross-correlated noise term correctly. Indeed, recent work suggests that a fully quantum mechanical theory is required to account properly for this term. This work is in collaboration with D. Kinion and supported by DOE BES.


3:42PM T3.00003 Optomechanics with microwave light, KONRAD LEHNERT, JILA: University of Colorado and NIST — Recently, superconducting circuits resonant at microwave frequencies have revolutionized the measurement of astrophysical detectors and superconducting qubits [2]. In this talk, I will describe how we extend this technique to measuring and manipulating nanomechanical oscillators. By strongly coupling the motion of a nanomechanical oscillator to the resonance of the microwave circuit we create structures where the dominant dissipative force acting on the oscillator is the radiation pressure of microwave “light” [3]. These devices are ultrasonic force detectors and they allow us to cool the oscillator towards its motional ground state.


4:18PM T3.00004 Noise in Mesoscopic, Quantum, and Nano-Systems, IRFAN SIDDIQI, University of California, Berkeley — Superconducting circuit elements can be used to form high quality factor harmonic and anharmonic oscillators. When coupled to a pseudospin system, these oscillators can be used for quantum state measurement. In the dispersive limit, the oscillator resonant frequency depends on the spin state. The case of a linear transmission line resonator coupled to a superconducting qubit was demonstrated by R. Schoelkopf and co-workers [1]. We will describe quantum measurement performed using a nonlinear resonator consisting of a Josephson tunnel junction shunted with a reactive impedance. The Josephson oscillator is excited with an increasing number of photons, its resonant frequency progressively decreases. Under appropriate bias conditions, it is also possible to access a bifurcation where two dynamical states exist. We will show that with a nonlinear Josephson oscillator, it is possible to realize both analog and digital quantum state measurement with variable gain. We will discuss two protocols for accessing the nonlinear response of the junction, amplitude modulation and frequency modulation, and describe in detail two applications—superconducting qubit readout and high speed magnetometry of single molecule magnets.


Wednesday, March 18, 2009 2:30PM - 5:30PM – Session T4 DCMP DAMOP: Polariton Condensates 306/307

2:30PM T4.00001 Theory of polariton condensation, PETER LITTLEWOOD, University of Cambridge — Lately, some novel experiments with planar optical microcavities make use of the mixing of excitons with photons to create composite bosons called polaritons that have a very light mass, and are thus a good candidate for high-temperature Bose condensation. Good evidence for spontaneous coherence has now been obtained. There are special issues to resolve, considering the effects of low dimensionality, disorder, strong interactions, and especially strong decoherence associated with decay of the condensate into environmental photons—since the condensate is a special kind of laser.

3:06PM T4.00002 Bose-Einstein Condensation of Microcavity Polaritons in Harmonic Traps. DAVID SNOKE, Department of Physics and Astronomy, University of Pittsburgh — Polaritons in microcavities are a two-dimensional, weakly interacting boson gas, and their spatial distribution, momentum distribution, coherence properties, and excitation spectrum can all be observed. In several recent experiments, these observations are consistent with the interpretation of a quasiequilibrium Bose condensate of polaritons. In our experiments, we use a special stress geometry to create a harmonic potential for the polaritons in the plane of their motion, which is analogous to the traps used in experiments on BEC of cold atoms. Among other effects, we observe coherent light emission from the polariton condensate. Two questions arise: 1) Since the system emits coherent light, how can we distinguish it from a standard laser? 2) How do we distinguish it from some type of nonlinear amplification of the excitation light? In our experiments with a trapping potential, we can easily distinguish between these different effects. We demonstrate two transitions which occur in the same place in the same structure, one which is standard lasing and one which is polariton condensation. The quasiequilibrium polariton condensate in microcavities thus emerges as a new type of coherent light emitter.

3:42PM T4.00003 Observation of Bogoliubov excitations in exciton-polariton condensates. YOSHIHISA YAMAMOTO, Stanford University — Particle-particle interaction and peculiar excitation spectra are keys for understanding BEC and superfluidity physics. A quantum field-theoretical formulation for a weakly interacting Bose condensed system was developed by Bogoliubov in 1947, which predicted the phonon-like excitation spectrum in the low-momentum regime. Exciton-polaritons in a semiconductor microcavity are elementary excitations created by strong coupling between quantum-well excitons and microcavity photons, were proposed as a new BEC candidate in solid-state systems. Recent experiments with exciton-polaritons have demonstrated several interesting signatures from the viewpoint of polariton condensation, such as quantum degeneracy at nonequilibrium densities, the polariton-bunching effect at the condensation threshold, long spatial coherence and quantum degeneracy at equilibrium conditions. The particle-particle interaction and the Bogoliubov excitation spectrum are at the heart of BEC and superfluidity physics, but have only been studied theoretically for exciton-polaritons. In this talk, we report the first observation of interaction effects on the exciton-polariton condensate and the excitation spectra, which are in quantitative agreement with the Bogoliubov theory.

4:18PM T4.00004 Quantum fluid dynamics and superfluid behaviour of polaritons in microcavities. DANIELE SANVITTO, Universidad Autonoma Madrid — Achievement of polariton condensation in semiconductor microcavities [1,2] has opened the way to the study of new interesting phenomena related to the behaviour of non-equilibrium Bose particles in the quantum limit. In this talk we will see the formation of a coherent quantum state of polaritons created at a given momentum and at a given time using a combination of a continuous wave pump and a pulsed probe. This state is observed to persist in the cavity for a time much longer than the cavity lifetime [3]. Using this technique we are able to investigate the behaviour of the quantum state of polaritons with an extension of ~ 20 µm moving a hundreds of monens within the cavity. One of the most striking effects of a moving polariton condensate is the observation of superfluid behaviour when crossing obstacles even at speeds only 100 times smaller than the speed of light [4]. Other interesting phenomena, which will be shown, are diffusion-less motion, due to the linearization of the polariton dispersion, and the formation of Cherenkov-like patterns for polaritons moving at supersonic velocities.

4:54PM T4.00005 Theory of polariton condensation and superfluidity1. ALEXEY KAVOKIN, University of Southampton — Exciton-polaritons in planar microcavities have two allowed spin projections on the axis of the structure, which is why they can be considered as a two-component weakly interacting Bose gas. The order parameter for BEC or the superfluid phase transition in this gas is a 2D vector analogous to the Jones vector of classical light. The build-up of the order parameter results is the build up of vector polarisation of light emitted by the polariton condensate. Recently observed near-field Cherenkov-like patterns for polaritons moving at supersonic velocities.


Wednesday, March 18, 2009 2:30PM - 6:06PM — Session T5 FIAP DBP: Industrial Biophysics 401/402

2:30PM T5.00001 Virus Characterization by FFF-MALS Assay. VLADIMER RAZINKOV, Amgen, Inc. — Adequate biophysical characterization of influenza virions is important for vaccine development. The influenza virus vaccines are produced from the allantoic fluid of developing chicken embryos. The process of viral replication produces a heterogeneous mixture of infectious and non-infectious viral particles with varying states of aggregation. The study of the relative distribution and behavior of different subpopulations and their inter-correlation can assist in the development of a robust process for a live virus vaccine. This report describes a field flow fractionation and multilayer light scattering (FFF-MALS) method optimized for the analysis of size distribution and total particle counts. A method using a combination of asymmetric flow field-flow fractionation (AFFFF) and multilayer light scattering (MALS) techniques has been shown to improve the estimation of virus particle counts and the amount of aggregated virus in laboratory samples. The FFF-MALS method was compared with several other methods such as transmission electron microscopy (TEM), atomic force microscopy (AFM), size exclusion chromatography followed by MALS (SEC-MALS), quantitative reverse transcription polymerase chain reaction (RT Q-PCR), median tissue culture dose (TCID(50)), and the fluorescent focus assay (FFA). The correlation between the various methods for determining total particle counts, infectivity and size distribution is reported. The pros and cons of each of the analytical methods are discussed.
3:06PM T5.00002 Determination of reversible protein equilibrium association coefficients using light scattering. MICHAEL LARKIN, Wyatt Technology Corporation — The characterization in solution of reversible protein associations as well as associations between proteins and small molecules is essential in many areas of science. Understanding cellular function or developing and formulating pharmaceuticals or other biologically active materials often requires quantitation of such associations. Most pharmaceuticals have functionality due solely to association with molecules within the body, and the discovery and accurate characterization of these associations is a key element for pharmaceutical development. Unfortunately, most methods used to measure associations of proteins require either immobilizing the protein on a surface (e.g. surface plasmon resonance), which potentially alters the protein characteristics, or require considerable time and effort and large quantities of sample (e.g. analytical ultracentrifugation, isothermal titration calorimetry). Light scattering based measurements of reversible association coefficients require much less sample and may be performed much more rapidly than other free solution techniques. In this talk I describe how static and dynamic light scattering may each independently be used to measure equilibrium association coefficients between proteins in free solution, and may also be used to observe and quantitate the association of small molecules with them. I present background theory for both static and dynamic light scattering measurements of equilibrium associations, and examples of measurements made of both model systems and of systems with commercial relevance in the pharmaceutical industry.

3:42PM T5.00003 Novel medical imaging technologies for disease diagnosis and treatment , DIEGO OLEGO, Philips Healthcare — New clinical approaches for disease diagnosis, treatment and monitoring will rely on the ability of simultaneously obtaining anatomical, functional and biological information. Medical imaging technologies in combination with targeted contrast agents play a key role in delivering with ever increasing temporal and spatial resolution structural and functional information about conditions and pathologies in cardiology, oncology and neurology fields among others. This presentation will review the clinical motivations and physics challenges in on-going developments of new medical imaging techniques and the associated contrast agents. Examples to be discussed are:

- The enrichment of computer tomography with spectral sensitivity for the diagnosis of vulnerable sclerotic plaque.
- Time of flight positron emission tomography for improved resolution in metabolic characterization of pathologies.
- Magnetic particle imaging -a novel imaging modality based on in-vivo measurement of the local concentration of iron oxide nano-particles - for blood perfusion measurement with better sensitivity, spatial resolution and 3D real time acquisition.
- Focused ultrasound for therapy delivery.

4:18PM T5.00004 Measurement Frontiers in Molecular Biology , STEPHEN LADERMAN, Agilent Laboratories, Agilent Technologies, 5301 Stevens Creek Blvd, Santa Clara, CA, 95051 USA — Developments of molecular measurements and manipulations have long enabled forefront research in evolution, genetics, biological development and its dysfunction, and the impact of external factors on the behavior of cells. Measurement remains at the heart of exciting and challenging basic and applied problems in molecular and cell biology. Methods to precisely determine the identity and abundance of particular molecules amongst a complex mixture of similar and dissimilar types require the successful design and integration of multiple steps involving biochemical manipulations, separations, physical probing, and data processing. Accordingly, today’s most powerful methods for characterizing life at the molecular level depend on coordinated advances in applied physics, biochemistry, chemistry, computer science, and engineering. This is well illustrated by recent approaches to the measurement of DNA, RNA, proteins, and intact cells. Such successes underlie well founded visions of how molecular biology can further assist in answering compelling scientific questions and in enabling the development of remarkable advances in human health. These visions, in turn, are motivating the interdisciplinary creation of even more comprehensive measurements. As a further and closely related consequence, they are motivating innovations in the conceptual and practical approaches to organizing and visualizing large, complex sets of interrelated experimental results and distilling from those data compelling, informative conclusions.

4:54PM T5.00005 Biophysics at the Boundaries: The Next Problem Sets , MALCOLM SKOLNICK — The interface between physics and biology is one of the fastest growing subfields of physics. As knowledge of such topics as cellular processes and complex ecological systems advances, researchers have found that progress in understanding these and other systems requires application of more quantitative approaches. Today, there is a growing demand for quantitative and computational skills in biological research and the commercialization of that research. The fragmented teaching of science in our universities still leaves biology outside the quantitative and mathematical culture that is the foundation of physics. This is particularly inopportune at a time when the needs for quantitative thinking about biological systems are exploding. More physicists should be encouraged to become active in research and development in the growing application fields of biophysics including molecular genetics, biomedical imaging, tissue generation and regeneration, drug development, prosthetics, neural and brain function, kinetics of nonequilibrium open biological systems, metabolic networks, biological transport processes, large-scale biochemical networks and stochastic processes in biochemical systems to name a few. In addition to moving into basic research in these areas, there is increasing opportunity for physicists in industry beginning with entrepreneurial roles in taking research results out of the laboratory and in the industries who perfect and market the inventions and developments that physicists produce. In this talk we will identify and discuss emerging opportunities for physicists in biophysical and biotechnological pursuits ranging from basic research through development of applications and commercialization of results. This will include discussion of the roles of physicists in non-traditional areas apart from academia such as patent law, financial analysis and regulatory science and the problem sets assigned in education and training that will enable future biophysicists to fill these roles.

5:30PM T5.00006 Characterizing Protein Complexes with UV absorption, Light Scattering, and Refractive Index Detection, STEVEN TRAINOFF, Wyatt Technology Corporation — Many modern pharmaceuticals and naturally occurring biomolecules consist of complexes of proteins and polyethylene glycol or carbohydrates. In the case of vaccine development, these complexes are often used to induce or amplify immune responses. For protein therapeutics they are used to modify solubility and function, or to control the rate of degradation and elimination of a drug from the body. Characterizing the stoichiometry of these complexes is an important industrial problem that presents a formidable challenge to analytical instrument designers. Traditional analytical methods, such as using fluorescent tagging, chemical assays, and mass spectrometry perturb the system so dramatically that the complexes are often destroyed or uncontrollably modified by the measurement. A solution to this problem consists of fractionating the samples and then measuring the fractions using sequential non-invasive detectors that are sensitive to different components of the complex. We present results using UV absorption, which is primarily sensitive to the protein fraction, Light Scattering, which measures the total weight average molar mass, and Refractive Index detection, which measures the net concentration. We also present a solution of the problem inter-detector band-broadening problem that has heretofore made this approach impractical. Presented will be instrumentation and an analysis method that overcome these obstacles and make this technique a reliable and robust way of non-invasively characterizing these industrially important compounds.

Wednesday, March 18, 2009 2:30PM - 5:30PM –
Session T6 FIP FGSA: Panel Discussion: Preparation of Graduate Students for Careers in a Globalized World
2:30PM T6.00001 Preparing for Change: Challenges and Opportunities in a Global World
SABINE O’HARA, Institute of International Education — Our world is becoming increasingly global. This may sound like a cliché, yet it is true nonetheless, and poses unprecedented challenges for graduate education. For the new generation of researchers, teachers and professionals to be successful they must be prepared in more than the content area of their chosen field. They must also acquire proficiency in global awareness, cultural literacy, multicultural teamwork and language facility. These global skill sets form the basis for effective multicultural collaboration and will become increasingly important even for those who do not intend to study or work abroad. Knowledge has become more portable in the internet age; large data bases and reports can be accessed in real time from various locations around the globe; information is exchanged in multifaceted knowledge networks; collaborative research takes place within and outside of the traditional venue of the research university in the private sector, research institutes, and associations; research networks span multiple disciplines as progress invariably occurs at the intersection of previously discrete fields of inquiry. Global collaboration thus is no longer dependent on the physical proximity of collaborators but can take place anywhere any time. This then requires yet another set of skills, namely the ability to adapt to change, exhibit flexibility and transfer skills to a range of contexts and applications. Effective graduate education must address these realities and expose students to learning opportunities that will enable them to acquire these much needed global skills sets.

3:06PM T6.00002 International Experiences for Graduate Students: Opportunities and Challenges, AMY FLATTEN, APS Director of International Affairs — Graduate students are often well aware that their physics careers may involve international partnerships at some point. Many students, however, wish to pursue international experiences during their graduate physics training. The speaker will discuss some of the international opportunities available to graduate students and provide insights into some potential challenges of engaging internationally.

3:30PM T6.00003 Graduate studies in a globalized world¹, FATIHA BENMOHKTAR, Carnegie Mellon — In our days physics research, experiment and theory, is done in one way or an other in a framework of an international collaboration. As an experimental Medium Energy physicist, I will be talking about my experience in working within international collaborations for more than twelve years. I will go through a couple of questions graduates students should be asking: How is the work environment for a graduate student doing his or her research within these collaborations? What about language barriers? Can they be independent in their analysis? What will happen after getting their PhD? — and more.

¹ Thanks to the APS

3:54PM T6.00004 Physics Internationally From the Industrial Perspective, T. VENKATESAN, National University of Singapore — Physicists traditionally get employed by academia, National Labs and industry. The investment of multi-national companies in R&D and manufacturing operations globally has been accelerating owing to availability of trained human resources and the economy of operation. This has created tremendous opportunities for candidates with global experience as opposed to a highly localized education. In the last decade, the investments made by Asian academic institutions in education and research and seen a significant increase creating opportunities for Graduate students and researchers alike in parts of the world other than US and Europe, the traditional destinations for students and researchers over the last several decades. Many Asian universities are hiring a diverse faculty from all over the world as opposed to hiring from local talent pools. Many of the Asian countries are focusing on creating local hitech economies by fostering global entrepreneurship programs. In my talk I will discuss this globalization phenomenon with specific examples from both academia and industry. I will also discuss strategies for academic institutions in terms of making the appropriate modification to their programs to deal with this inevitable evolution.

4:18PM T6.00005 I2CAM and ICAM: Physics Internationally, DANIEL COX, University of California Davis — The Institute for Complex Adaptive Matter (I2CAM) through the National Science Foundation sponsored International Institute for Complex Adaptive Matter (ICAM) has, since its formal inception in 2002, grown into a 60+ branch international scientific network devoted to the study of emergent phenomena in correlated electron matter, soft matter, and biological matter. We conducts forefront research through a blend of discussion oriented workshops (at least 50% of the time for discussion), exchange awards for junior scientists to initiate collaborations between two groups, travel awards for junior scientists to present research work or carry out brief research, and schools on topical subject matter. We also supplement our federal funding with contributions from each branch which support postdoctoral and senior scientist fellowships and unique science outreach activities such as an online science museum (The Emergent Universe). We have also outreach activities to universities with substantial numbers of underrepresented groups in the sciences and to outstanding science institutes in emerging nations. We will review what has worked well with I2CAM/ICAM, how we started and grew, and how we have inspired similar programs in other countries. (This research supported by NSF Grants DMR-0645461 and DMR-0456669).

4:42PM T6.00006 Panel Discussion —

Wednesday, March 18, 2009 2:30PM - 5:30PM – Session T7 GSNP DPOLY: Patterns on Thin Elastic Sheets 407

2:30PM T7.00001 The undulating shape of growing ribbons, HAIYI LIANG, School of Engineering and Applied Science, Harvard University — The undulating morphology of leaves and petals is now accepted as a consequence of differential growth of the underlying tissue. Various qualitative and quantitative aspects of the buckling patterns seen in both vascular and avascular leaves may thus be ascribed to the distribution of non-uniform growth in the lamina, and have been demonstrated in normal and mutant leaves, as well as in physical models thereof. To understand the different modalities that arise quantitatively, we construct a mathematical model for the stability of an initially flat or curved elastic ribbon with gradients in growth directly motivated by observations of kelp that are capable of phenotypic plasticity in different environments. Using a combination of analysis, numerical simulation, and experimental observations, we map out the phase space of possible shapes for these growing ribbons. In general, we find that as the relative growth strain is increased, the ribbon-like structure first switches to a catenoidal shape before developing undulating edges that can develop on the catenoid’s edges. Our framework allows us to delineate the few macroscopic parameters that control the morphology of elongated leaves and flower petals and helps to explain the large variety of observed shapes.

3:06PM T7.00002 The Mechanics of Non-Euclidean Plates in Synthetic and Natural Sheets, ERAN SHARON, The Hebrew University of Jerusalem — Thin elastic flat plates attain non-trivial configurations when they are confined. I will show that plates with intrinsic non-Euclidean geometry attain multi scale three-dimensional configurations even when they are free of external loading. Such bodies do not have any stress-free configuration, thus current plate theories cannot properly describe their physics. I will present our recent experimental results and our theoretical model for the shaping principles of such plates. Finally, I will show how these principles are manifested during the growth of leaves.
3:42PM T7.00003 Wrinkling patterns on floating elastic films\footnote{1}, NARAYANAN MENON, Dept. of Physics, University of Massachusetts, Amherst — A polymer sheet floating on the surface of a fluid is an ideal arena for studying elastic instabilities in thin sheets. In our experiments we use polystyrene sheets whose typical lateral size, $L \sim 3 \text{ cm}$, and whose thickness, $t$ ranges from 30 to 300 nm, yielding aspect ratios $L/t$ of up to $10^3$. In their unperturbed state, they lie on the surface of a pool of water, stretched flat by surface tension. We can then generate a rich variety of wrinkle patterns by perturbing the surface locally with capillary forces or with controlled displacements at one or more points on the surface. I will review our understanding of the length scales that characterise these localised patterns. A simple experimental setting in which a multiplicity of these length scales come into play is a situation analogous to an Euler buckling experiment performed on the surface of a fluid. We push two sides of a rectangular sheet towards each other, creating a global pattern of parallel wrinkles whose wavelength is given by a balance between gravitational potential energy of the fluid and bending energy of the sheet. These wrinkles develop a cascade of fine structure at higher wavenumbers close to the uncompressed edges of the sheet. The length scale over which this cascade occurs is the capillary length, whereas the wavenumber at the edge of the sheet reflects a balance between bending energy and surface tension. We discuss the evidence that this is a fundamentally new type of elastic cascade, which proceeds to higher wavenumbers by smooth evolution of the wrinkles, rather than by discrete, sharply localised branching. Work done in collaboration with J. Huang, E. Cerda, B. Davydovitch, W.H. de Jeu, T.P. Russell, C. D. Santangelo

1Supported by NSF DMR 0606216 and NSF MRSEC DMR-0820506.

4:18PM T7.00004 Wrinkle to fold transitions: Stress relaxation in lipid monolayers and other elastic thin films, KA YEE C. LEE, The University of Chicago — Surfactants at air/water interfaces are often subjected to mechanical stresses as the interfaces they occupy are reduced in area. The most well characterized forms of stress relaxation in these systems are first order phase transitions. However, once chemical phase transitions have been exhausted, the monolayer undergoes global mechanical relaxations termed collapse. We have previously demonstrated that for lung surfactants, a mixture of lipids and proteins that coats the alveol of the airway, the collapse process occurs at an in-plane rigidity. We characterize the rigidity of the monolayer by analyzing in-plane morphology on numerous length scales. More rigid monolayers collapse out-of-plane via a hard elastic mode similar to an elastic membrane, with the folded state being the final collapse state, while softer monolayers relax in-plane by shearing. For the hard elastic mode of collapse, we have further demonstrated experimentally and theoretically that the folded state is preceded by a wrinkled state, and similar wrinkle to fold transitions has been observed in elastic thin films ranging from 2 nm to 10 $\mu$m in thickness of completely different chemical nature (lung surfactant lipid monolayers, gold nanoparticle trilayers, and polyester sheets).

4:54PM T7.00005 Nonlinear dynamics of wrinkle growth and pattern formation in stressed elastic thin films on viscoelastic substrates, RUI HUANG, University of Texas at Austin — A stressed thin film on a soft substrate can develop complex wrinkle patterns. The onset of wrinkling and initial growth is well described by a linear perturbation analysis, and the equilibrium wrinkle patterns can be analyzed based on an energy approach. In between, the wrinkle pattern undergoes a growth and coarsening process with a peculiar dynamics. By using a proper scaling along with numerical simulations, this paper develops a quantitative understanding of the wrinkling dynamics from initial growth through coarsening toward equilibrium. By considering generally biaxial stresses and anisotropic elastic modulus of the film, we show that a rich variety of wrinkle patterns (e.g., labyrinth, orthogonal, parallel, zigzag, and checkerboard patterns) emerge as a result of the competition between the material anisotropy and the stress anisotropy.

Wednesday, March 18, 2009 2:30PM - 5:30PM – Session T8 DCMP: Onsager Prize, Nicholson Medal, Apker Award, Davison-Germer Prize 414/415

2:30PM T8.00001 Nicholson Medal Talk: Hydrodynamic Turbulence , KATEPALLI SREENIVASAN, International Centre for Theoretical Physics, Trieste, Italy — This talk will be an introduction on hydrodynamic turbulence to a non-specialist audience. It will summarize the essential developments in the field, and only modest emphasis will be placed on the speaker's own work. Hydrodynamic turbulence may be said to have begun as a subject of scientific study with Osborne Reynolds' classical paper towards the end of the nineteenth century, but it is a subject of great interest in the 21st century. The intent is to highlight the principal accomplishments in a way that draws attention to their connections to other areas of physics, where possible.

3:06PM T8.00002 Lar Onsager Prize Talk: An Exactly soluble model for Strontium Copper Borate: Mott Hubbard Physics on an Archimedean Lattices\footnote{1}, SRIRAM SHASTRY, University of California Santa Cruz — An exactly soluble model of spin half particles on a certain 2-dimensional frustrated lattice has been recently realized in the compound $\text{SrCu}_2(\text{BO}_3)_2$, and other similar systems have been found more recently. These systems appear to be ideal testing grounds for contemporary theoretical ideas on the role of correlations and frustration in Mott Hubbard systems. In this talk I will summarize the work on these systems emphasizing their role in testing key concepts.

1The speaker acknowledges support from NSF-DMR-0706128 and DOE-BES DE-FG02-06ER46319.

3:42PM T8.00003 LeRoy Apker Award Talk: Electronics at the Nanoscale: Graphene, Carbon Nanotubes, and Single-Molecule Devices , SUJIT DATTA, Department of Physics, Harvard University — Low-dimensional nanostructures are emerging as model systems for fundamental studies of quantum transport, as well as promising candidates for novel post-silicon electronic devices incorporating quantum size effects. Key examples of these include few-layer graphene, carbon nanotubes, polymer nanofibers, and even single molecules. In this talk, I will summarize my work combining experimental and computational tools to study, control, and apply molecular nanomaterials of low dimensionality — using scanning probe microscopy techniques to study electronic phenomena in few-layer graphene and carbon nanotubes, as well as to elucidate the structure of biochemically-functionalized carbon nanotubes; using computer simulations to investigate key electronic properties of single-molecule transistors; and demonstrating a straightforward chemical technique by which samples of few-layer graphene can be etched along their crystallographic directions, potentially enabling the creation of a variety of new graphene-based nanostructures.
4:18PM T8.00004 Davisson-Germer Prize Talk: Hydrogen storage in nanoporous materials. YVES CHABAL, University of Texas at Dallas — To develop a hydrogen-based energy technology, several classes of materials are being considered to achieve the DOE targets for gravimetric and volumetric hydrogen densities for hydrogen storage, including liquids (e.g. ammonium borohydrides), clathrate structures, complex metal hydrides, nanostructured (e.g. carbon) nanoporous materials. Fundamental studies are necessary to determine the ultimate hydrogen capacity of each system. Nanoporous Metal-organic Framework (MOF) materials are promising candidates for hydrogen storage because the chemical nature and size of their unit cell can be tailored to weakly attract and incorporate H2 molecules, with good volumetric and mass density. In this talk, we consider the structure M2(BDC)2(TED), where M is a metal atom (Zn, Ni, Cu), BDC is benzenedicarboxylate and TED triethylene diamine, to determine the location and interaction of H2 molecules within the MOF. These compounds are isoostructural and crystallize in the tetragonal phase (space group P4/nnc), they construct 3D porous structures with relatively large pore size (~7-8 Å^-1), pore volume (~0.63-0.84 cc/g) and BET surface area (~1500-1900 m^2/g). At high pressures (300-800 ps), the perturbation of the H-H stretching mode can be measured with IR absorption spectroscopy, showing a 35 cm^-1 redshift from the unperturbed ortho (4155 cm^-1) and para (4161 cm^-1) frequencies. Using a newly developed non empirical van der Waals DFT method vdW-DFT, it can be shown that the locus of the deepest H2 binding positions lies within to types of narrow channels. The energies of the most stable binding sites, as well as the number of such binding sites, are consistent with the values obtained from experimental adsorption isotherms, and heat of adsorption data. Importantly, the calculated shift of the H-H stretch is ~30 cm^-1, at the strongest binding points of the two channels, suggesting that the combination of IR and vdW-DFT gives a consistent and accurate picture of H2 binding in MOF structures. These methods can therefore provide the fundamental information necessary to guide synthesis for improving H2 uptake and release. 

1 This work was supported by the grant DOE-DE-FG02-08ER46491, and performed in collaboration with N. Nijem (UTD), and L. Kong, V. Cooper, K. Li, J. Li and D.C. Langreth (Rutgers University)

4:54PM T8.00005 Davisson-Germer Prize Talk: Surface vibrations of adsorbates on Si(111): From small clusters to infinite lattices. KRISHNAN RAGHAVACHARI, Indiana University — Organic functionalization of semiconductor surfaces is a growing research area that offers the possibility of molecular level control of surface features and tailored electronic properties. In this work, quantum chemical cluster calculations are used in conjunction with surface vibrational spectroscopy to determine the structures of functionalized Si(111) surfaces. Interestingly, the interpretation of these spectra even for simple adsorbates is not straightforward. In the limit of high coverage, most calculations using small cluster models lack the long range coupling of the real surface that is required to make definitive assignments. In order to understand the relationship between clusters and infinite periodic vibrations, we have investigated the geometries and harmonic vibrational frequencies of the methyl, acetylenyl, methacetylenyl, hydrogen, deuterium and chlorine functionalized Si(111) surfaces. From a careful analysis of these systems, we have derived a technique where the collective vibrational modes corresponding to the vibrations of the infinite periodic system can be derived from relatively small cluster models. The calculated frequencies are in good agreement with available experimental values and yield novel insights about the coupling between low frequency adsorbate frequencies and surface phonons. The efficacy of this approach for surfaces of varying adsorbate coverage and the prediction of novel frequency shifts will be discussed along with more complex systems.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T9 GSNP: Focus Session: Stochastic Processes in Biological Systems I 303

2:30PM T9.00001 Stochastic models of viral infection. TOM CHOU, UCLA — We develop biophysical models of viral infections from a stochastic process perspective. The entry of enveloped viruses is treated as a stochastic multiple receptor and coreceptor engagement process that can lead to membrane fusion or endocytosis. The probabilities of entry via fusion and endocytosis are computed as functions of the receptor/coreceptor engagement rates. Since membrane fusion and endocytosis entry pathways can lead to very different infection outcomes, we delineate the parameter regimes conducive to each entry pathway. After entry, viral material is biochemically processed and degraded as it is transported towards the nucleus. Productive infections occur only when the material reaches the nucleus in the proper biological state. Thus, entry into the nucleus in an infectious state requires the proper timing of the cytoplasmic transport process. We compute the productive infection probability and show its nonmonotonic dependence on both transport speeds and biochemical transformation rates. Our results carry subtle consequences on the dosage and efficacy of antivirals such as reverse transcription inhibitors.

3:06PM T9.00002 Stochastic modeling of gene regulation by small RNAs. VLAD ELGART, Department of Biology, Virginia Tech, TAO JIA, ANDREW FENLEY, RAHUL KULKARNI, Department of Physics, Virginia Tech — Recent research has uncovered several examples wherein post-transcriptional regulation by small RNAs plays an important role in critical cellular processes. We considered a stochastic model for regulation of target mRNAs by small RNAs. While the corresponding master equation is analytically intractable, application of the bursty synthesis approximation of the Gillespie algorithm and to the results of linear noise approximation approach. The effects of transcriptional pulsing on protein steady-state expression are also explored within the same formalism.

3:18PM T9.00003 Stochastic modeling of protein-based post-transcriptional regulation. TAO JIA, RAHUL KULKARNI, Virginia Tech — Recent experiments have enabled monitoring gene expression in living cells at the level of single proteins. Data from such experiments for protein burst-size distribution and burst frequency can be used to obtain analytical expressions for the steady-state protein distribution across a population. We extend this analysis to the case of modulation of gene expression by binding/unbinding of a post-transcriptional regulatory protein. Closed-form analytical expressions and results from stochastic simulations will be presented. In the case that regulator binding results in complete repression of protein expression, the steady-state protein distribution has the same functional form as the unregulated case, once the mRNA degradation rate is appropriately renormalized. For the general case, wherein binding can result in partial repression or even activation of protein expression, we derive an analytical expression for the steady-state distribution which generalizes the result for the unregulated case.

3:30PM T9.00004 Accurate fluctuation prediction in epidemics using stochastic model reduction. ERIC FORGOSTON, IRA SCHWARTZ, U.S. Naval Research Laboratory — We consider a large-scale dynamical system with stochastic forcing and outline a general theory to reduce the dimension of the stochastic system. The general procedure employs a stochastic normal form coordinate transform and allows one to analytically derive both the stochastic center manifold and the reduced set of stochastic evolution equations. The transformation correctly projects both the dynamics and the noise onto the center manifold. We have applied the theory to a stochastic Susceptible-Exposed-Infected-Recovered (SEIR) epidemiological model. When compared with the original model, the reduced dynamical system accurately predicts fluctuations of disease outbreaks both in amplitude and phase.

1 Research supported by the Office of Naval Research and the Army Research Office.
3:42PM T9.00005 Stochastic disease extinction in multistrain diseases with interacting strains

SIMONE BIANCO, LEAH SHAW, The College of William and Mary, IRA SCHWARTZ, Naval Research Laboratory — The study of multistrain diseases, diseases with several coexisting strains, is a major challenge for mathematical biology. Examples of such diseases are influenza, HIV, dengue, and ebola. In this work we present an agent-based model for multistrain diseases with strain interactions mediated by antibody-dependent enhancement. An individual infected with a strain develops antibodies which will protect him/her against all the strains. When the level of protection wanes, the presence of antibodies will enhance the infectiousness of the individual when an infection with a different strain occurs. This mechanism is called antibody-dependent enhancement (ADE). We use this model to investigate the role that fluctuations due to system size have on disease extinction paths and discuss how interactions mediated by ADE affect rates of disease fade-out. Finally, we discuss the effect that varying the number of strains has on disease extinction.

3:54PM T9.00006 Controlling rare events: optimizing disease extinction with limited vaccine

M. KHASIN, M.I. DYKMAN, Michigan State University — In rare events such as switching between stable states or disease extinction the system has to overcome an effective barrier. The barrier height can be changed by the effective change of a control field. The change is determined by the effective work of the field along the most probable trajectory followed in a rare event. In turn, the barrier change results in an exponentially strong change of the event rate. We study the optimal temporal shape of the control field with a constraint that the time-average field value and the sign of the field are fixed. An example is vaccination with a limited vaccine production rate or control by light intensity with a limited laser power. For a comparatively weak field, for a broad class of rare events, optimal control is accomplished by periodically applying δ-like pulses. We show that the barrier change may display resonant dependence on the pulse period and is linear in the pulse area. For a stronger field, the dependence of the barrier change on the field amplitude becomes system-dependent. The results are applied to simple models of population dynamics.

4:06PM T9.00007 Extinction Time Distribution in Stochastic Lotka-Volterra System

MATTHEW PARKER, ALEX KAMENEV, University of Minnesota — The Lotka-Volterra model is one of the most basic problems in population dynamics. The mean-field solution to this problem predicts oscillatory evolution of two competing populations. However, an account of the discrete nature of agents inevitably results in the extinction of one or both species. We studied the distribution function of times required for such an extinction event to take place. We employed a combination of Monte-Carlo simulations and analytic techniques. As a result we achieved a complete understanding of the distribution function in the limiting cases of long and short extinction times. The long time tail is perfectly described by the lowest eigenvalue of the corresponding Fokker-Planck operator. Moreover, due to time scale separation, one may reduce the initial 2D operator to an effective 1D radial one. Remarkably, in the short time limit the Fokker-Planck approach fails, and one has to resort to the WKB treatment of the full evolution operator of the corresponding discrete stochastic problem.

4:18PM T9.00008 Refined mean-field approaches to “edge-effects” in open TASEP’s

JIAJIA DONG, Hamline University, ROYCE K.P. ZIA, BEATE SCHMITTMANN, Virginia Tech — We study the totally asymmetric simple exclusion process (TASEP) with a defect site, hopping rate \(q < 1\), at the edge of the system and particles occupying \(l\) lattice sites. Using two different mean-field approximations, we analyze the behavior of the steady state current \(J\) in the presence of the defect as a function of entry rate \(\alpha\) and \(q\). In good agreement with Monte Carlo simulations, these two methods bring insight to understanding the significance of having one or a cluster of slow codons (unit of messenger RNA, template of protein synthesis) immediately after initiation during protein synthesis. Related work is published in Journal of Physics A, vol. 41 (2008).

4:30PM T9.00009 Parallel Coupling of Symmetric and Asymmetric Exclusion Processes

KONSTANTINOS TSEKOURAS, Rice University, ANATOLY KOLOMEISKY, Rice University Chemistry Department — A system consisting of a simple symmetric exclusion process (SSEP) and a totally asymmetric exclusion process (TASEP) coupled to each other at every site is constructed as a simplified model of a microtubule and the surrounding medium within the context of intracellular particle transport. Transitions between the channels are allowed at every site of both lattices. A cluster-based mean-field theory allows calculation of stationary phase diagrams, particle currents and densities for symmetric/asymmetric transition rates between the channels. It is shown that in general there are three stationary phases, similar to the case of a single-channel totally asymmetric exclusion process. Density profiles are identical in both channels if transition rates are symmetric, not so if they are asymmetric. At certain limiting values of the transition rates our theory provides exact solutions, so that the system can be described as a partially asymmetric exclusion process (PASEP). Extensive Monte Carlo simulations generally support theoretical predictions, although simulated stationary-state properties slightly deviate from calculated in the mean-field approximation. Dynamic properties and phase diagrams are discussed by analyzing symmetry requirements and constraints on the particle currents, as are possible implications for the problem of intracellular particle transport.

4:42PM T9.00010 Anomalous diffusion and scaling in the dynamics of coupled stochastic processes

GOLAN BEL, CNLS and CCS-3 LANL, ILYA NEMENMAN, CCS-3 and CNLS LANL — Stochastic processes are ubiquitous in nature, and multiple dynamical variables in the same physical system can be stochastic simultaneously. Common mathematical treatment of such cases limit the interactions among multiple stochastic variables to simple correlations. However, more complicated couplings are possible as well. For example, for many biochemical reactions, the rate (stochastic) of creation of one substance may depend on the presence of another one, itself stochastic variable. Here we present a theoretical study of one class of such coupled stochastic processes. We observe that, contrary to traditional modeling frameworks, even very weak coupling yields anomalous diffusion. Interestingly, the diffusion exponent cannot be predicted by simple scaling arguments, and anomalous scaling appears as well. Further, we show that even weak inhibitive coupling between the two processes may result in dynamics equivalent to that of the celebrated comb model, where the coupling between the two stochastic variables is so strong that one is able to diffuse only when the other is within a certain range. We compare the model to various mechanisms for generating anomalous diffusion and show that coarse-graining yields behavior equivalent to that of the non-ergodic continuous time random walk. We end with brief discussion of applications of the developed theory to biochemical systems.

4:54PM T9.00011 Subdiffusion in the Internal Dynamics of Peptides

THOMAS NEUSIUS, Computational Molecular Biophysics, IWR, University of Heidelberg, Im Neuenheimer Feld 368, D-69120 Heidelberg, JEREMY C. SMITH, Center for Molecular Biophysics, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge TN 37831-6164 — The internal dynamics of biopolymers is a topic of intense current research, both in experiment and theory. Recent experimental results have demonstrated the presence of internal subdiffusion in biopolymers at equilibrium. Molecular dynamics simulation of oligopeptide chains reveals configurational subdiffusion at equilibrium extending from 10^{-12} to 10^{-6} s. We examine the possible origins of the subdiffusion and demonstrate that it arises from the fractal-like structure of the accessible configurational space [PRL 100, 188103 (2008)].
5:06PM T9.00012 Stochastic waiting times of complex biochemical reactions may exhibit universal behavior. B. MUNKSKY, G. BEL, N. SINITSYN, I. NEMENMAN, Los Alamos National Lab — To model cell regulatory pathways, one must understand the complex nature of these pathways. We investigate the behavior of biochemical reactions in complex networks and show that the universal behavior of these reactions can be described by a set of equations.

5:18PM T9.00013 Mechanisms of high energy plasmon modes in thin films. MATTHEW B. SMITH, DICHIOMIOS VAVYLOIS, Department of Physics, Lehigh University — We investigate the surface plasmon modes of a thin metallic film using the Plasmon Hybridization method. We find that the high energy modes are related to the bonding and antibonding modes of the surface plasmon.

Wednesday, March 18, 2009 2:30PM - 5:30PM Session T10 DMP: Focus Session: Optical Properties of Nanostructures V: Plasmonics and Metamaterials 304

2:30PM T10.00001 Metal films with arrays of subwavelength holes show infrared spectral and plasmonic sensitivity to material in the holes. JAMES COE, JOSEPH HEER, KATHERINE CILWA, MARVIN MALONE, LLOYD CORWIN, The Ohio State University — We investigate the infrared absorption spectra of metal films with arrays of subwavelength holes. The results show that the material in the holes has a significant effect on the plasmonic response.

2:42PM T10.00002 Influence of the dielectric environment on periodic hole arrays. DIMITRIOS KOUKIS, DANIEL J. ARENAS, SINAN SELCUK, DAVID B. TANNER, ARTHUR F. HEBARD, SERGEI V. SHABANOV — We study the effect of the dielectric environment on the plasmonic response of metal films with periodic hole arrays. We find that the dielectric environment can significantly affect the plasmonic response.

2:54PM T10.00003 Controlling the polarization of light transmitted through metallic bilayers of subwavelength apertures. ZSOLT MARCET, J. PASTER, H.B. CHAN, University of Florida, D.W. CARR, Symphony Acoustics, J.E. BOWER, R. CIRELLI, F.P. KLEMEMS, W.M. MANSFIELD, J.F. MINER, C.S. PAI, J.A. TAYLOR, Bell Labs, I. KRAVENCHKO, Oak Ridge National Laboratory — We investigate the polarization of light transmitted through metallic bilayers of subwavelength apertures. We find that the polarization can be controlled by the design of the bilayers.

3:06PM T10.00004 Perfect coupling of light to surface plasmons with ultra-narrow linewidths. MAXIM SUKHAREV, Arizona State University, PAUL SIEVERT, TAMAR SEIDEMAN, JOHN KETTSSONER, Northwestern University — We examine the coupling of electromagnetic waves to surface plasmons in thin metallic films. We find that the coupling can be made ultra-narrow.

3:18PM T10.00005 Plasmon Hybridization of a thin metallic film. TAE-HO PARK, PETER NORDLINDER, Department of Physics and Astronomy, Rice University — We investigate the plasmon modes of a thin metallic film using the Plasmon Hybridization method and solving Maxwell’s equations. We show that the high energy plasmon mode is the antibonding mode in which surface charges are antisymmetrically distributed, and the low energy mode is the bonding mode in which surface charges are symmetrically distributed. In the thin film, secondary charges which are induced from the primitive plasmons on the other film surface play an important role to determine which plasmon mode has the higher or lower energy. Furthermore, we discuss how the secondary charges affect the propagation length of the surface plasmon by calculating the imaginary parts of the surface plasmon wave vectors.
3:30PM T10.00006 Plasmon coupling in nanoparticle rings, STEPHAN LINK, WEI-SHUN CHANG, LIANE SLAUGHTER, BISHNU KANAL, PRAMIT MANNA, EUGENE ZUBAREV — A surface plasmon is excited when the conduction band electrons of a metal oscillate coherently in phase with incoming excitation light. Plasmons can exist and propagate along structures that are smaller than the diffraction limit of light, the parameter which currently dictates the minimum size of optical interconnects. In addition to exploiting plasmons on continuous structures like thin films and nanowires for waveguiding, arrays of nanoparticles also pose potential for waveguiding. We have characterized the plasmon coupling of self-assembled rings of 40 nm gold nanoparticles functionalized with polystyrene using dark-field scattering microscopy and spectroscopy. Comparing images and spectra from the rings to those of single particles together with correlating images acquired by dark-field and SEM microscopy, we observe redshifted coupled plasmon modes that show a strong polarization dependence. In particular, segments of the ring aligned parallel to the axis of detected polarization display higher order longitudinal plasmon modes, similar to those observed for a long rod.

3:42PM T10.00008 Transforming Light with Metamaterials, VLADIMIR SHALAEV, Purdue University — Metamaterials are expected to open a gateway to unprecedented electromagnetics properties and functionality unattainable from naturally occurring materials, thus enabling a family of new “meta-devices.” We review this new emerging field and significant progress in developing metamaterials for the optical part of the spectrum. Specifically, we describe recently demonstrated artificial magnetism across the whole visible, negative-index in the optical range, and promising approaches along with challenges in realizing optical cloaking. A new paradigm of engineering space for light with transformation optics will be also discussed.

4:30PM T10.00009 Analytic LC model for plasmonic resonances in nano-structured split-ring resonators, P. W. KOLB, Laboratory for Physical Sciences, College Park, MD 20740, T. D. CORRIGAN, A. B. SUSHKOV, H. D. DREW, D. C. SCHAMDEL, Department of Physics, University of Maryland, College Park, MD 20742, R. J. PHANEUF, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742 — We systematically investigate the plasmonic resonant behavior of metallic nano-structured split-ring resonators as a function of the size of the split gap, substrate permittivity, metal skin depth, and sample height. We performed simulations of the structures and examine the E-field and current density maps. We present a simple, analytic LC model to describe the lowest order resonance and its dependence on the aforementioned parameters.

4:42PM T10.00010 Angular Dependence of Resonances from Rod Pairs and U-Shapes, TIMOTHY CORRIGAN, University of Maryland, PAUL KOLB, Laboratory for Physical Sciences, ANDREI SUSHKOV, DENNIS DREW, DOMINIC BRITTI, RAYMOND PHANEUF, University of Maryland — We examine and compare the angular dependence of electric and magnetic resonances from rod pairs and U-shapes made of Ag with the long arms placed both horizontally and vertically. We discuss the results in terms of photonic band structure effects. In addition, we observe that the splitting of the higher order mode for vertical U-shapes in the s-polarization behave as symmetric and anti-symmetric modes in which the modes red and blue shift, respectively, as observed previously. However, both horizontal U-shapes and rod pairs also show a split for the p-polarization in which both modes red shift. We discuss the reasons for this behavior using both experimental results and simulations.

5:06PM T10.00012 Natural negative refraction index in polycrystalline Fe and Ni at optical frequencies, ADIL-GERAI KUSSOW, Dept. of Physics, University of Massachusetts Lowell, ALKIM AKYURTU, Electrical and Computer Engineering Dept., University of Massachusetts Lowell — Analysis of the photon-magnon interactions in Fe and Ni, 3d transition-metal ferromagnetics, demonstrating the coupling between the incident light and high-frequency spin waves with energy (0.2 – 0.35) eV is presented. As a consequence, these metals in their polycrystalline form with nanoscale grains are found to possess a negative refraction index at optical frequencies, close to the high-frequency ferromagnetic resonance. The effect is due to the coexistence of the spin wave mode with the plasmonic mode, and both modes are activated by the e.m. field of the light, with simultaneous permittivity and permeability responses within some frequency band.

5:18PM T10.00013 Propagating and Localized Surface Waves in Metamaterial Stacks, RUWEN PENG, YONGJUN BAO, ZHAOHUI TANG, FENG GAO, ZHIJIAN ZHANG, WEIHUA SUN, XIN WU, MU WANG, National Laboratory of Solid State Microstructures, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES TEAM — We demonstrate the interference effect between propagating and localized modes of electromagnetic wave in metamaterial stacks, which leads to a transmission extremum. When radiation is incident on a metal surface perforated with an array of ring-shaped subwavelength apertures, the phase difference between the propagating surface Bloch wave and the localized surface wave can be tailored by the geometrical parameters of the array so as to affect the shape of the transmission spectrum. Above the resonant frequency of the aperture, interference between the surface waves leads to a minimum in the transmission spectrum, whereas below it, the interference leads to a maximum. While in multiple metamaterial stacks with hole arrays, the coupling of surface electromagnetic wave yields a new resonant mode with increasing quality factor of the transmission peak. We suggest that these features provide flexibility in engineering surface wave-based all-optical devices. Reference: Y. J. Bao, R. W. Peng, D. J. Shi, Mu Wang, X. Lu, J. Shao, W. Lu, and N. B. Ming, Phys. Rev. Lett. (2008) 101, 087401.

1Supported by NSF and MOST in China.
2:30PM T11.00001 Platform for Measurement of Phonon Scattering from the Surface of Silicon Nanostructures. J. P. SULLIVAN, Sandia National Labs, T. A. FRIEDMANN, E. S. PIEKOS, S. L. SHINDE, J. R. WENDT — We’ve created a micro-platform for measuring thermal phonon surface scattering in single-crystal Si nanostructures, specifically specular-to-diffuse surface scattering in the long phonon mean-free-path regime. The platform consists of three suspended co-linear monocrystalline Si islands with the center island resistively heated and connected to its neighbors by Si nanoligaments (one ligament straight, the other bent). The ligaments have a blade-like geometry with length, width, and depth of 1000 nm, 100 nm, and 2500 nm, respectively. Heat conducts from the center island across the ligaments in proportion to the ligament thermal conductance, which is lower for the bent ligament due to increased surface scattering. Monte Carlo simulations indicate that the heat flux differs between straight and bent nanoligaments by 10% for diffuse (rough surface) phonon reflection and by almost 40% for specular (smooth surface) reflection. Acknowledgment: DOE BES Div. of Mat. Sci. & Eng. and LDRD (Sandia is operated by Sandia Corp. for the US DOE’s NNSA, contract DE-AC04-94AL85000).

2:42PM T11.00002 Thermal Effects in Precision Nano-Electronics Construction, STEPHEN JOHNSON, SON, OSCAR D. RESTREPO, KALMAN VARGA, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and ORNL — Mobility is a key factor in charge transport since it describes how the motion of an electron is affected by an applied electric field. As such, it is an important element in the design of new devices. Mobilities are generally modeled using methods that suppress atomic-scale detail (effective mass theory or bulk energy bands for electron velocities, empirical deformation potentials, macroscopic roughness, etc.). Parameter fitting to experimental data is needed. As new technologies require modeling of transport at the nanoscale and new materials are introduced, predictive parameter-free mobility modeling is needed. The main scattering mechanisms that limit mobilities are due to phonon, ionized impurities, and interface roughness. A first-principles calculation of mobilities limited by atomic scale roughness with atomic-scale detail was reported recently [1]. We report the development of parameter-free quantum-mechanical methods to calculate scattering rates and electron mobilities limited by phonon and ionized-impurity scattering in a self-consistent way. Results for n-doped silicon are in good agreement with experimental data. This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005).

2:54PM T11.00003 First-principles parameter-free calculations of electron mobilities in silicon: phonon and Coulomb scattering , OSCAR D. RESTREPO, KALMAN VARGA, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University and ORNL — Mobility is a key factor in charge transport since it describes how the motion of an electron is affected by an applied electric field. As such, it is an important element in the design of new devices. Mobilities are generally modeled using methods that suppress atomic-scale detail (effective mass theory or bulk energy bands for electron velocities, empirical deformation potentials, macroscopic roughness, etc.). Parameter fitting to experimental data is needed. As new technologies require modeling of transport at the nanoscale and new materials are introduced, predictive parameter-free mobility modeling is needed. The main scattering mechanisms that limit mobilities are due to phonon, ionized impurities, and interface roughness. A first-principles calculation of mobilities limited by atomic scale roughness with atomic-scale detail was reported recently [1]. We report the development of parameter-free quantum-mechanical methods to calculate scattering rates and electron mobilities limited by phonon and ionized-impurity scattering in a self-consistent way. Results for n-doped silicon are in good agreement with experimental data. This work was supported by NSF Grant ECS-0524655. [1] M. H. Evans et al., Phys. Rev. Lett. 95, 106802 (2005).

3:06PM T11.00004 Reconstructing Fourier’s law from disorder in quantum wires1. MASSIMILIANO DI VENTRA, YONATAN DUBI, University of California - San Diego — The validity of Fourier’s law in nano-scale wires poses a fundamental theoretical challenge, with both scientific and technological implications. In this work, a novel theory of open quantum systems is used to study the local temperature and heat currents in metallic nanowires connected to leads at different temperatures. We show that for ballistic wires the local temperature is almost uniform along the wire and Fourier’s law is invalid. By gradually increasing disorder, a uniform temperature gradient ensues inside the wire and the thermal current linearly relates to this local temperature gradient, in agreement with Fourier’s law. Finally, we show that while disorder is responsible for the onset of Fourier’s law, the non-equilibrium energy distribution function is determined solely by the heat baths.

1Work supported by the DOE.

3:18PM T11.00005 A Single-Molecule Phonon Field-Effect Transistor, MARCOS MENEZES, Universidade Federal do Rio de Janeiro, Brazil, BRENDA MOREIRA, Universidade Federal do Pará, Brazil, JORDAN DEL NERO, Universidade Federal do Pará and Universidade Federal do Rio de Janeiro, Brazil, RODRIGO CAPAZ, Universidade Federal do Rio de Janeiro, Brazil — Controlling phonons in the same way we control electrons in materials has been an old but elusive dream for physicists. In particular, it would be extremely desirable to control the thermal (phonon) flux between two reservoirs using a gate electric field, i.e., to construct a field-effect transistor for phonons. However, in most materials, electric fields do not couple strongly to lattice vibrations. Moreover, at the molecular and nano scale, in which the ballistic regime is dominant, thermal conductance of acoustic modes is universal, independent of the sound velocity. Therefore, modulating the sound velocity does not change the thermal conductance, thus making even more difficult the conception of such device. In this work, we propose a realizable architecture for a phonon field-effect transistor based on a single polar polymeric molecule placed between two reservoirs. An applied transverse electric field transforms the acoustic torsion mode into optical. For feasible temperatures and electric field magnitudes, this coupling can virtually suppress the contribution from this mode to the thermal conductance, therefore modulating the conductance by as much as 25%.

3:30PM T11.00006 Hypersonic Phononic Crystal Based on 2D Single Crystalline Nanoporous Alumina, AKIHIRO SATO, Max Planck Institute for Polymer Research, YAN PENNEC, Institut d’Electronique, de Microélectronique et de Nanotechnologie, TAKASHI YANAGISHITA, Tokyo Metropolitan University, BAHRAM DJAFARI-ROUHANI, Institut d’Electronique, de Microélectronique et de Nanotechnologie, FYTAS GEORGE, F.O.R.T.H Institute of Electronic Structure and Laser Technology, WOLFGANG KNOLL, Max Planck Institute for Polymer Research, HIDEKI MASUDA, Tokyo Metropolitan University — Periodic nanocomposite media consisted of alumina matrix and infiltrated cylindrical nanopores exhibit rich elastic wave propagation behaviour including the localization of phonons, anisotropic propagation and the formation of phononic band gaps at GHz frequencies. We have examined the translational symmetry dependence of dispersion relations on 2D single crystalline phononic crystals based on nanoporous alumina using Brillouin light scattering. The propagation of elastic waves is significantly different between native and filled with fluids alumina matrix. For the latter, the dispersion relations become independent of the propagation direction, as opposed to the native alumina scaffold. Theoretical band diagrams and the displacement fields describe well the experimental results.
3:42PM T11.00007 Charge Carrier Confinement in a Nano-patterned Silicon Film

ZHENG LIU, Dept. of Material Science and Engineering, U. of Utah, Salt Lake City, UT, 84112 & Center for Advanced Study, Tsinghua Univ., Beijing, China, 100084, WENHUI DUAN, Department of Physics, Tsinghua University, Beijing, China, 100084, FENG LIU, Department of Material Science and Engineering, University of Utah, Salt Lake City, Utah, 84112, JIAN WU, Department of Physics, Tsinghua University, Beijing, China, 100084 — Impurity scattering is becoming a critical problem in sub-micrometer MOSFET. One way to reduce the impurity scattering is by separating carriers from dopants, as used in the modulation-doping technique. From first-principles calculation, we find that by etching channels along (001) direction on the surface of a thin (110) silicon film, the hole states can be strongly confined in the film underneath the patterned layer. Therefore, by selective doping in the top patterned layer, a modulation-doping-like effect can be achieved, which is expected to greatly enhance the hole mobility. This effect arises from matching between carrier wavefunction orientation and quantum confinement direction determined by film and pattern geometry. It will be functional as long as the patterned feature size is within a few nanometers.

1This work was supported by the Ministry of Science and Technology of China (Grants No. 2006CB605105 and 2009CB929401), the Ministry of Education of China, and National Natural Science Foundation of China (Grants No. 10674078 and 10721404).

3:54PM T11.00008 Magnetotransport of Bi nanowires: Evidence for surface carriers in bismuth,

TITO HUBER, Howard University, ALLA NIKOLAEVA, LEONID KONOPKO, Academy of Sciences Moldova, MICHAEL J. GRAF, Physics Department. Boston College. — Angle resolved photoemission spectroscopy studies (Hirahara et al, Phys. Rev. Lett. 97, 146803 (2006)) provide evidence of quantum-confined bulk-like states and surface states in ultrathin Bi films. Can these states be observed in electronic transport? We studied magnetotransport of trigonal Bi nanowires (30 nm < diameter < 200 nm) for fields up to 14 T. Bulklike states (M.R. Black et al. Phys. Rev. B68, 235417 (2003)) are identified because of its anisotropic Fermi surface and low effective mass. A two-dimensional behavior was expected of high-effective mass surface carriers; we found instead a three-dimensional behavior, with a rich spectrum of Landau levels in a nearly spherical Fermi surface. This behavior is related to the long penetration length of surface states on non-basal surfaces. On the basis of similarity of spectra, we show that recent observations of sharp peaks in the bulk Bi Nernst thermopower near the 9 T quantum limit, attributed to charge fractionalization (K. Behnia, L. Balicas and Y. Kopelevich, Science 317, 1729 (2007)), can be more plausibly interpreted in terms of quasiparticles that are based on surface states. Bismuth true quantum limit is 70 T.

1High Magnetic Field Laboratory, Wroclaw. Poland. NSF-DMR.

4:06PM T11.00009 Nanoscale Charge Transport in Realistic Organic Thin-Films: Beyond Variable-Range Hopping and Percolation Networks

GEOFFREY HUTCHISON, University of Pittsburgh, Department of Chemistry, MARCUS HANWELL, XIALING CHEN, AARON CRANDALL. — We are building up experimental and computational model systems for charge transport in nanoscale organic electronic devices. In particular, our combined approach is aimed at addressing questions as to the effect of impurities, traps, and other defects on electronic conductivity. Experimentally, we have designed thin films and monolayers to which we can controllably add known quantities of defects with known electronic properties. In tandem, we focus on a new Monte Carlo style simulation of charge transport in these imperfect devices with an aim to move beyond simple variable-range hopping models. Our goal is to establish all parameters for our simulations from first-principles calculations and detailed experimental results. I will describe initial results and comparisons with other organic electronic materials and existing charge transport models.

4:18PM T11.00010 Computational Simulation of Charge Transport in Metal Terpyridine Monolayer FETs

MARCUS HANWELL, GEOFFREY HUTCHISON, University of Pittsburgh — Understanding the roles of charge traps and defects in electronic transport in organic materials is becoming increasingly important. Computational studies have been undertaken, using an agent-based Monte Carlo method, of the active region of a monolayer FET. Charge transport is assumed to be due to thermally activated, variable-range hopping between neighboring sites. This model system allows us to probe the role of charge traps/defects both computationally and experimentally. We do this by using multiple metal terpyridine complexes, each having known electronic structure. Using Marcus Theory and quantum calculations, the hopping rate between neighboring complexes can be predicted. Results from computational simulations of this system will be discussed, with special attention being paid to the results that can be experimentally verified, such as voltage-current curves.

4:30PM T11.00011 Random telegraph noise and low frequency noise in molecular tunnel junctions

DOMINIQUE VUILLAUME, NICOLAS CLEMENT, DAVID GUERIN, STEPHANE PLEUTIN, IEMN-CNRS, DAVID CAHEN, Weizmann Institute — Molecules of organic molecules present one of the main systems studied in molecular electronics. We report the observation and study of a low frequency noise and Random Telegraph Signal (RTS) in self-assembled alkyl chain junctions on silicon. The 2 levels of current can be clearly distinguished. With a sufficiently long recording time (> 500 events), statistics can be performed on the current level and on the upper and lower times. The RTS amplitude is usually few % of the average current and the process follows poissonian statistics. This RTS signal is also modulated by another RTS with a much longer time constant. This allowed us evaluation of the change of noise in the frequency domain from 1/f noise to Lorentzian like spectrum. In inorganic tunnel junctions, such signal can only be observed in sub-micrometric junctions whereas we observe it in almost millimetric junctions. This precludes mechanisms involving electron trapping / detrapping in single isolated trap. We propose several hypotheses leading to long-range fluctuations including molecular dynamics and relaxation processes.

4:42PM T11.00012 Maximum energy transfer in nanoscale thermal radiation

SOUMYADIPTA BASU, ZHUOMIN ZHANG, Georgia Institute of Technology — Radiation heat transfer between closely spaced objects has received much attention lately because of the emerging applications of near-field thermophotovoltaics, thermal radiation scanning tunneling microscopy, and nanothermal manufacturing. The energy transfer in nanoscale radiation can exceed that of blackbody radiation by several orders of magnitude due to photon tunneling and the excitation of surface polaritons. An outstanding question remains as whether there exists an upper limit of near-field radiation for arbitrarily selected material properties. We examine the maximum radiative energy flux between two parallel plates separated by a vacuum gap from 0.1 and 100 nm distance. An upper bound is imposed to the parallel wavevector component in the analysis based on fluctuational electrodynamics. By assuming a frequency-independent dielectric function, we find that the maximum heat flux depends on the chosen complex permittivity and the distance. The determination of the achievable heat flux at nanometer distances will benefit future research and applications of near-field radiation for energy harvesting.

1This work was supported by the Department of Energy under contract number DE-FG02-06ER46343.
2:30PM T12.00001 Atomic structures and energetics of methanol and its reaction intermediates on the ZnO(0001) surface: A first-principles study, KATAWUT CHUSASIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHY STAMPFL, University of Sydney — Methanol (CH₃OH) is widely used in various chemical synthesis, and in particular it is predicted to be one of the next generation of renewable energy sources as a fuel for fuel cells. Industrially, methanol is mass produced by A₂O₂-supported Cu/ZnO catalysts. However, the role of ZnO in the methanol synthesis is still unclear. To provide a better understanding of the mechanisms underlying this process, we present first-principles total-energy calculations of the methanol molecule and its reaction intermediates on the ZnO(0001) surface. A detailed characterization of atomic geometries and associated energetics is presented. The reaction intermediates we consider are CH₃O, CH₂O, HCOOH, HCOO, HCO, H₂O, CO₂, CO, OH and H. These intermediate species are reported from experimental studies to be present during methanol decomposition on the ZnO(0001) surface. We also analyse the vibrational frequencies of each of the adsorbed fragments. The information obtained will be used for investigating the surface chemical reactions of associated with methanol synthesis over the ZnO surface.

2:42PM T12.00002 Morphology of alloy catalysts in an oxidizing environment: Structure-sensitivity of ethylene epoxidation over Ag-Cu particles, SIMONE PICCININ, CATHERINE STAMPFL, University of Sydney, MATTHIAS SCHEFFLER, Fritz-Haber-Institut — Ag-Cu alloys have been proposed as catalysts for ethylene epoxidation due to their superior selectivity compared to pure silver, the predominant catalyst for this reaction [1]. By means of density-functional theory and atomistic thermodynamics, we study the surface structure and morphology of Ag-Cu particles in thermodynamic equilibrium with an oxygen atmosphere. Contrary to the common assumption of the formation of a 2D surface alloy, we find that at temperatures and pressures of interest for practical applications the particles can display a variety of structures, including thin Cu-surface oxides in coexistence with clean Ag. At variance with pure Ag in UHV, we find that under reactive conditions the (111) facet is not dominant. We identify different reaction pathways that will compete and/or synergetically interplay in the catalysis. In general, the reaction mechanism is structure-dependent and often the reaction does not proceed through the formation of stable intermediates, in contrast to clean Ag and the 2D alloy. Analyzing the competing reactions, we discuss how the addition of Cu improves the selectivity and stress the overall importance of accounting for the effect of ambient conditions. [1] S. Linic et al. J. Catal. 224, 148 (2004)

2:54PM T12.00003 Interaction of benzene and MMA vapors with TiO₂ surface: Relevance to EUV Lithography¹, BORIS YAKHINSKIY, SHIMON ZALKIND, ROBERT BARTYNSKI, Rutgers University — We characterize the surface processes that affect the reflectivity and lifetime of TiO₂ — capped multilayer mirrors used in EUV lithography. Low energy electron beam is used to mimic excitations initiated by EUV radiation. Temperature programmed desorption, x-ray photoelectron spectroscopy, and low energy ion scattering are used to analyze the surface reactions. Carbon film growth on TiO₂ (001) crystalline surface is measured during electron bombardment in benzene or MMA vapor (model background gases) over a wide range of pressures and temperatures near 300 K. The surface temperature, gas pressure and electron energy are shown to be important for growth of carbon. The substrate temperature rise lowers the carbon accumulation rate. Increasing the vapor pressure over the surface enhances the carbon deposition, and variation of the electron energy shows a pronounced influence on the reaction rate. Low energy secondary electrons excited by EUV photons contribute substantially to carbon accumulation on clean TiO₂ cap layers. The steady-state coverage of the molecules on the surface and the cross-sections for electron-stimulated dissociation are key parameters for understanding and modeling the processes on the EUVL mirrors.

¹This work is supported by Intel.

3:06PM T12.00004 Selective Oxidation of Ammonia on RuO₂(110): a combined DFT and KMC study¹, SAMPYO HONG, Univ. of Central Florida, ALTAF KARIM, Brookhaven National Laboratory, SERGEY STOLBOV, TALAT RAHMAN, Univ. of Central Florida — Motivated by the experiments of Wang et al [1] on the selective oxidation of ammonia on RuO₂(110), we have performed first principles electronic structure calculations based on the density functional theory (DFT) and the pseudopotential method to calculate the activation energy for the associated reaction processes, and used the DFT results in kinetic Monte Carlo (KMC) simulations of the reaction rates. We find the overall energy barriers for NH₃ + O₂ = N₂ + H₂O, N₂ + O₂ = NO₂, and N₂ + O = NO to be about 1.0, 0.6, and 0.56 eV, respectively. We also find, in agreement with experiment, intermediate products such as NH to be short-lived (i.e. not detectable in experiment). For a simple model of the surface dominated by the two end reactions above, our KMC simulations show almost 100% selectivity toward NO, in excellent agreement with experimental findings. For more realistic simulation, in which we include several intermediates and their reactions (over 20 processes), KMC simulations show about 60% selectivity toward NO within the experimental O₂ pressure range. We compare our calculated reaction rates to those obtained in experiment and rationalize our results through details of the surface electronic structure. [1] Y. Wang, K. Jacobi, W.-D. Schoene, and G. Ertl, J. Phys. Chem. B 2005, 109, 7883-7893.

¹Work supported in part by DOE DE-FG02-07ER15842.

3:18PM T12.00005 Surface Chemistry of Cyanogen on Copper, EREVERE LEE, JAMES LALLO, ERIK CIFTLIKLI, SYLVE RANGAN, ALEXEI ERMAKOV, B.J. HINCH, Rutgers University — The surface chemistry of cyanogen/cyanide species has been observed on Cu(100) crystal through Temperature Programmed Desorption, Helium Atom Scattering and soft x-ray Photoelectron Spectroscopy. Cyanogen (CN₂) dissociates on copper to form a mixture of cyanide and cyanogen (CN) species depending at cryogenic temperatures but pure cyanide at ambient temperatures, leading to c(10x6) superstructure in two domains at saturation. Temperature Programmed Desorption spectra observed indicated that cyanide recombinatively desorbs as cyanogen at relatively high temperatures with no additional species observed. The desorption results were analysed using a variety of techniques in order to determine the activation energy of desorption (Ed) as well as its coverage dependency.

3:30PM T12.00006 Identifying surface intermediates with TPD: Methylchlorosilanes on Cu(001), JAMES LALLO, EREVERE LEE, B.J. HINCH, Rutgers University, DAN STRONGIN, Temple University — Various methylchlorosilane molecules (SiH₃MeₓClₙ₋ₓ, x+y+z=4) were exposed to a Cu(001) surface. Dissociative adsorption was observed for all hydrogen containing species, at surface temperatures above 160K. The chemistry and thermal stability of the surface bound fragments were then studied as a means for understanding intermediates of the commercially important “Direct Process,” namely production of Cl₂(CH₃)₂Si, from Si and CH₃Cl, with a Cu catalyst. Temperature programmed desorption indicates that methyl groups are readily transferred among adsorbed Si-containing species. A large fraction of Cl remains on the surface after observation of typically 2 or 3 distinct TPD features below 450K. By a comparison of the product species distributions to the parent species, we are then able to propose key intermediates common to many of the adsorption/desorption mechanisms.
3:42PM T12.00007 Surface-catalyzed O2 adsorption on quantum thin films , JSUN KIM, ALEXANDER KHAJETOORIANS, The University of Texas at Austin, WENGUANG ZHU, ZHENYU ZHANG, Oak Ridge National Laboratory & University of Tennessee, CHIH-KANG SHIH, The University of Texas at Austin — Pure crystalline Pb is well known to be inert with respect to oxygen gas. By using scanning tunneling microscopy we demonstrate that the oxygen adsorption on Pb films is greatly increased by Cs adsorbates acting as catalysts. Our previous studies show that Cs atoms can be easily incorporated into the surface layer of thin Pb films grown on Si(111). In addition, Cs adsorbates are able to adjust the surface energy so as to initiate stable Pb nanolands on Pb flat tops of unstable thickness. Because of this unique property Cs adsorbates on originally inert Pb films, they are a natural choice of template to investigate surface catalysis of quantum thin films. Bare Pb films do not oxidize until much higher coverage (1000L), but in the presence of Cs we see adsorption of oxygen at much lower exposures of only a few Langmuir. The oxidation first occurs preferentially at sites of Cs adsorption. After oxygen clusters nucleate, oxidation of the Pb film increases in proportion to the amount of oxygen exposure. During this process the formation of oxygen clusters forces changes in the film morphology. First-principles density functional theory calculations of the O binding energies on the alloyed surface layers will be done and compared with experiment.

3:54PM T12.00008 First principle studies of the oxygen reduction reaction on the CrN electrocatalyst , SERGEY STOLBOV, University of Central Florida — These fuel cells offer great advantages for various applications, but severe obstacles remain to their large scale implementation. The Pt-based catalysts, used in both electrodes make them unacceptably expensive. Furthermore, the low rate of the oxygen reduction reaction (ORR) on the Pt cathode significantly reduces efficiency of the device. In this work, ORR on alternative CrN electrocatalyst has been studied from first principles. It is found that, in contrast to Pt, oxygen molecules dissociate spontaneously on the CrN surfaces, which switch on simple 1-electron reduction mechanism. Based on the adsorption energy calculations the free energies of intermediates were obtained as functions of the electrode potential. This diagram explain a relatively high rate of ORR obtained experimentally [1] for this material. The effects of coverage and co-adsorbates have been also studied.

4:06PM T12.00009 Hydrogen Reduction at Room Temperature of Partially Oxidized Co Cluster Films Capped with Pd 1 , A. L. CABRERA, J. I. AVILA, R. TRABOL, Pontificia Universidad Catolica de Chile, C. ROMERO, M. J. VAN BAEL, P. LIEVENS, Katholieke Universiteit Leuven — Co clusters with mean size of 1.8 nm were deposited on sapphire substrates at 25°C, 300°C and 500°C respectively. They were capped by a continuous 15 nm Pd film. Visible light transmission and reflection, in the range 400 to 900 nm, were measured when the samples were exposed to different hydrogen pressures up to 130 Torr. D.C. electrical resistance of the films was also measured as an independent property of the films to confirm hydrogen absorption by the samples. In all the samples the transmission and reflection of the films increased, reaching saturation at around 35-40 Torr hydrogen pressure. The relative change in the resistance of all Co cluster samples is smaller than the change in pure Pd films, indicating that hydrogen absorption is limited to the Pd capping layer only. We observed a significant decrease in the transmittance and the resistance during the first hydrogenation cycle of the sample prepared at 25°C suggesting that a reduction of the partially oxidized Co clusters occurred at room temperature.

4:18PM T12.00010 H2 dissociation of H2 on Co layers on Cu(111) from abinitio studies 1 , DUY LE, SERGEY STOLBOV, TALAT RAHMAN, University of Central Florida — Through first principles electronic calculations, based on the spin-polarized density functional theory using the generalized gradient approximation and the ultrasoft pseudopotential method in the plane wave representation, we studied the adsorption and the dissociation of H2 on two Co layers grown on Cu(111). As H2 approaches the surface with the H-H bond parallel to that surface, it dissociates at a distance of about 1.7Å from the Co layer, and constituent H atoms proceed to occupy neighboring fcc and hcp sites. The "adsorption" energy barrier for H2 is 0.14 eV and the "dissorption" energy is about 0.80eV. On the Co surface, H diffuses from an fcc site to an hcp site, or vice versa, with diffusion barriers of 0.17eV and 0.12eV respectively. We find no evidence of subsurface H. By analyzing the local electronic density of state, we establish, in agreement with suggestion from experiments [1], that the surface electronic states and magnetic moment of Co atoms depend very much on the H coverage.

4:30PM T12.00011 Structural and catalytic properties of thin CeO2 films on TiO2 substrate , I.G. BATYREV, ARL. Adelphi, MD, N.S. RASHKHEV, INL, Idaho Falls, ID — Structural properties of CeO2(111) thin films on top of a TiO2(110) substrate have been investigated by first-principles calculations. We found the special orientation of the ceria film relative to the rutile substrate that corresponds to a small (few percent) lattice mismatch between the two oxide surfaces. The positions of interfacial Ti atoms undergo some structural modulations during the relaxation process. Also, the relaxation of the interface resulted in the appearance of elongated Ce-O bonds at some sites of the O-terminated surface of CeO2/TiO2 films. These oxygen sites at the surface show low activation energy for loosing oxygen atoms and, therefore, they have higher catalytic activity in CO oxidation by the Mars-van Krevelen mechanism. We predict from the simulations that higher rate of the catalytic CO oxidation should have CeO2(111)/TiO2(110) films compared with CeO2(111) surface, which may also be attributed to the elongation of Ce-O bonds at some sites of O-terminated film in comparison with a pure ceria surface. We discuss the role of oxygen vacancies in the CO oxidation at reduced films and investigate the interplay between migration of O bulk atoms to the surface O vacancy sites and the structural phase transition from the CeO2(111) (Ce4+ and Ce2O3(0001) (Ce2+) structures. This work was supported by the U. S. Department of Energy Contract DE-AC07-051D14517.

4:42PM T12.00012 Adsorption and Dissociation of Molecular Hydrogen on the (0001) Surface of DHCP Americium 1, PRATIK DHOLABHAI 2, ASOK RAY, The University of Texas at Arlington — Hydrogen molecule adsorption on the (0001) surface of double hexagonal closed packed americium has been studied in detail within the framework of density functional theory. Weak molecular hydrogen adsorption were observed. The most stable configuration corresponded to a Hor2 approach molecular adsorption at the one-fold top site where the molecule’s approach is perpendicular to a lattice vector. Adsorption energies and adsorption geometries for different adsorption sites will be discussed. The change in work functions, magnetic moments, partial charges inside muffin-tins, difference charge density and density of states for the bare Am slab and the Am slab after adsorption of the hydrogen molecule will be discussed. Reaction barrier for the dissociation of hydrogen molecule will be presented. The implications of adsorption on Am 5f electron localization-delocalization will be summarized.

1Work supported in part by DOE under Grant No DE-FG02-07ER46354.

2This work is supported by the U. S. Department of Energy and the Welch Foundation, Houston, Texas.

Current affiliation: Arizona State University
4:54PM T12.00013 Atomic Thermodynamic Approach for Determining Cu Catalyst Morphologies Under Reactive Water-Gas-Shift Conditions. NILAY INOGLU, JOHN KITCHIN, Dept. of Chemical Engineering, Carnegie Mellon University — The water gas shift reactions (WGS) are widely used in several industrial processes and are catalyzed by Cu catalysts. In coal derived syngas, there are sulfur (S) impurities which can adsorb on the Cu surfaces and block the active sites of the catalyst and can result in catalyst deactivation. The sulfur adsorption will compete with other possible adsorbates such as CO, O, H and CO$_2$ making a quantitative estimate of the impact of sulfur on reactivity difficult. To determine the interactions between these possible adsorbates with Cu, the adsorption properties of these different adsorbates on low Miller index facets of Cu surfaces were studied in the limit where these surfaces are in thermodynamic equilibrium with the reactive environment. The effect of S adsorption on the surface electronic structure was significant and coverage dependent. In addition to a site-blocking deactivation mechanism, we found that sulfur modifies the surface electronic structure in a way that makes the Cu less reactive. Our results show that the adsorbates play a key role in defining the catalyst morphologies. We conclude that the presence of sulfur and other reactive adsorbates can impact the reactivity of the catalysts through several mechanisms including site-blocking, surface electronic structure modification and changes in the distribution and types of reactive sites through catalyst morphology changes.

5:06PM T12.00014 The nonlocal correlation as the solution of the CO puzzle problem. PREDRAG LAZIC, FZJuelich, Germany; MOJTABA ALAEI, Isfahan University of Technology, Iran; NICOLAE ATODIRESEI, Osaka University, Japan, VASILE CACIU, FZ Juelich, Germany; RADOVAN BRAKO, Rudjer Boskovic Institute, Croatia; STEFAN BLUEGEL, FZ Juelich, Germany — For the last 20 years the Density Functional Theory (DFT) has been the standard approach for the calculation of chemisorption, adsorption, chemical reactions and electronic structure in general. Despite the great successes of the theory in predicting adsorption energies and other properties for many systems it turns out that the theory fails to predict correctly the adsorption site preference for the CO molecule on (111) surfaces of Pt, Cu and Rh, for example. The DFT calculations predict that the highly coordinated FCC (hollow) site adsorption is preferred over the top site adsorption, while experiments show unambiguously that CO adsorbs into the top site. Also, the calculated adsorption energies do not match well the experimental values. CO molecule chemisorption on these surfaces is a type of system in which one would expect DFT theory in its present implementation with semi-local (GGA) functionals to work well. We show that the inclusion of the nonlocal correlation into the DFT calculations of CO chemisorption through vdW-DF functionally largely solves the discrepancies known as the CO puzzle problem.

5:18PM T12.00015 ABSTRACT WITHDRAWN — Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T13 DCOMP: Electronic Structure 309

2:30PM T13.00001 Three-dimensional statistical reduction of the non-relativistic Schrödinger equation for electrons with pair-wise Coulomb interactions. BOYAN OBRESHKOV, Arkansas University, Fayetteville, AR 72701, USA — Based on Ritz variational principle, we reduce in statistical fashion the non-relativistic Schrödinger equation for electrons with Coulomb interactions to a three-dimensional wave-equation for the motion of one electron with the residual $N - 1$ electrons acting spectators of its motion [1]. As a consequence the Pauli’s exclusion principle is interpreted as dynamical principle. Analytic solutions of the all electron quantal equations for the ground and excited states of the helium and lithium isoelectronic sequences will be represented and the comparison with the experimental measurements for the ground-state ionization potentials of atoms shown. [1] B. D. Obreshkov, Phys. Rev. A 78, 032503 (2008).

1Supported by NERSC Arkansas-Okahoma.

2:42PM T13.00002 High Pressure Phases of Cu$_2$O. DAVID GROH, Gannon U, RAVI PANDEY, Michigan Technological U, MIGUEL BLANCO, Universidad de Oviedo — Copper Oxide’s ambient phase is cubic. The copper atoms are in a simple face centered cubic packing sequence of hexagonal layers, with the oxygen atoms at alternating tetrahedral sites. As the pressure increases, cubic symmetry breaks. While the basic packing sequence is maintained, the distance between layers is no longer cubic — a hexagonal structure results. At even higher pressures, a major crystal structure change occurs to the CdI$_2$ structure. The calculated phase change pressures and volumes tend to compare well with experiment.

2:54PM T13.00003 k · p formalism within FLAPW method. TATSUYA SHISHIDO, TAMIO OGUCHI, Hiroshima University — We provide a k · p formalism within the full-potential linearized augmented plane wave (FLAPW) method. Unlike the pure plane waves, the LAPW functions do not behave trivially in moving from k to k+q and their incompleteness as a basis set should be taken into account. Derivatives of the sphere matching coefficients play the key role, for which we find a simple formula. Concrete formula for the k · p matrix elements is derived and numerically tested. Generalized second-order perturbation theory allowing for a degenerate case is presented and the literally-exact electronic band gradients and curvatures are accessible.

3:06PM T13.00004 Electric polarization in a Chern insulator. SINISA COH, DAVID VANDERBILT, Rutgers University — We extend the Berry-phase concept of polarization to insulators having a non-zero value of the Chern invariant. The generalization to such Chern insulators requires special care because of the partial occupation of chiral edge states. We show how the integrated bulk current arising from an adiabatic evolution can be related to a difference of bulk polarizations. We also show how the surface charge can be related to the bulk polarization, but only with a knowledge of the wavevector at which the occupancy of the edge state is discontinuous. We conclude by presenting numerical calculations on a model Hamiltonian to provide additional support for our analytic arguments.

3:18PM T13.00005 A new Laplacian representation for real-space calculations of general periodic and partially periodic systems. AMIR NATAN, AYELET BENJAMINI, DORON NAVEH, LEEOR KRONIK, Weizmann Inst of Sci, MURILO TIAGO, SCOTT BECKMAN, JAMES CHELIKOWSKY, University of Texas, WEIZMANN INST OF SCI TEAM, UNIVERSITY OF TEXAS TEAM — We present a real-space method for electronic-structure calculations of systems with general full or partial periodicity. The method is based on the self-consistent solution of the Kohn-Sham equations, using first principles pseudopotentials, on a uniform three-dimensional non-Cartesian grid. Its efficacy derives from the introduction of a new generalized high-order finite-difference ire Laplacian that avoids the numerical evaluation of mixed derivative terms and results in a simple yet accurate finite difference operator. Our method is further extended to systems where periodicity is enforced only along some directions (e.g., surfaces), by setting up the correct electrostatic boundary conditions and by properly accounting for the ion-electron and ion-ion interactions. Our method enjoys the main advantages of real-space grid techniques over traditional plane-wave representations for density functional calculations, namely, improved scaling and easier implementation on parallel computers, as well as inherent immunity to spurious interactions brought about by artificial periodicity. We demonstrate its capabilities on bulk GaAs and Na for the fully periodic case and for a monolayer of Si-adsorbed polar nitrobenzene molecules for the partially periodic case.
3:30PM T13.00006 Confinement effects on excitation energies and regioselectivity as probed by the Fukui function and the molecular electrostatic potential, ALEX BORGOO, Vrije Universiteit Brussel, DAVID TÖZER, Durham University, PAUL GEERLINGS, FRANK DE PROFT, Vrije Universiteit Brussel — When a molecule is placed as a guest inside a zeolite pore, its electronic structure will be altered, among others by the effect of the so-called “confinement”. It has been established that the compression of the molecular orbitals influences a system’s reactivity. In this work we use a simple potential barrier method to quantify the importance of confinement effects on chemical reactivity. In the first part, excitation energies and molecular orbital energy gaps are evaluated for molecules placed in cavities of different sizes. Our results for ethylene and formaldehyde reveal an increase in excitation energy and the gap between the occupied and the unoccupied levels. In the case of the larger molecules naphthalene and anthracene, the HOMO-LUMO gap shows very little sensitivity to the confinement. To investigate the role of confinement effects on local aspects of chemical reactivity and on regioselectivity, we evaluated its effect on the Fukui function and the molecular electrostatic potential, reaction indices that are central in the description of orbital and charge controlled reactions. The results indicate that confinement can influence the regioselectivity and that the reactivity of anions is expected to change, due to the artificial binding of the exess electron.

3:42PM T13.00007 Maximally-localized Wannier functions for GW quasiparticles, D. R. HAMANN, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — Recent efforts carrying the GW many-body approximation to self-consistency have given improved electronic structure results. Maximally-localized Wannier functions formed from the quasiparticle wave functions provide an efficient and highly accurate basis for interpolating the SCGW bands from a coarse Brillouin-zone mesh to symmetry lines. Since the MLWF’s correspond to chemists’ bond orbitals, they potentially also provide insight into the qualitative effects of the improved treatment of correlations in SCGW compared to LDA. We report results on SrTiO$_3$, solids Ar, and molecular CO. Band interpolation is accurate and effective for both solids. Small shifts in the degree of hybridization can be visualized for some of the SrTiO$_3$ and CO MLWF’s. In Ar, individual conduction-band Bloch functions were found to have large differences between LDA and SCGW. However, a manifold of 9 d and spd-hybrid MLWF’s which proved to be the minimum necessary for the lower conduction bands showed minimal differences in the two cases. A fully-functional interface to the WANNIER90 library within the SCGW-capable ABINIT code has been implemented and will be publicly available in the near future. 1. F. Brunval et al., Phys. Rev. B 74, 045102 (2006). 2. N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12 847 (1997). 3. M. van Schilfgaarde et al., Phys. Rev. Lett. 96, 226402 (2006).

3:54PM T13.00008 High-performance computational condensed-matter physics in the cloud, J. J. REHR, L. SVEC, J. P. GARDNER, M. P. PRANGE, U. of Washington — We demonstrate the feasibility of high performance scientific computation in condensed-matter physics using cloud computers as an alternative to traditional computational tools. The availability of these large, virtualized pools of compute resources raises the possibility of a new paradigm for scientific research with many advantages. For research groups, cloud computing provides convenient access to reliable, high performance clusters and storage, without the need to purchase and maintain sophisticated hardware. For developers, virtualization allows scientific codes to be pre-installed on machine images, facilitating control over the computational environment. Detailed tests are presented for the parallelized versions of the electronic structure code SIESTA and for the x-ray spectroscopy code FEFF, including CPU, network, and I/O performance, using the the Amazon EC2 Elastic Cloud.

1Supported by NSF DMR-0848950

4:06PM T13.00009 A scalable algorithm for the computation of Hartree-Fock exchange, IVAN DUCHEMIN, FRANCOIS GYGI, University of California Davis, Davis CA 95616 — Electronic structure calculations based on hybrid density functionals require efficient algorithms for the computation of the Hartree-Fock exchange operator. The high computational cost of Hartree-Fock exchange currently limits the use of such functionals in large-scale First-Principles Molecular Dynamics applications. We present a scalable parallel algorithm for the computation of Hartree-Fock exchange in a plane-wave, pseudopotential framework, with applications to electronic structure calculations of liquid water and various nanostructures. Technical issues arising in the implementation of hybrid density functionals will be discussed.

1Supported by NSF OCI 0749219 and DOE-SciDAC DE-FC02-06ER25794

4:18PM T13.00010 Compact representations of Kohn-Sham invariant subspaces, FRANCOIS GYGI, University of California Davis, Davis CA 95616 — We present a method to compute a hierarchical approximate representation of the solutions of the Kohn-Sham equations. The approach is based on a recursive bisection algorithm and yields one-particle wavefunctions localized on domains of varying sizes. The accuracy of the representation is set a priori by specifying the maximum error in the form of the approximate wavefunctions. Applications to the electronic structure of large systems are used to illustrate the data reduction achieved by this representation. The achievable data compression is similar to that obtained by truncating Maximally Localized Wannier Functions. Implications for the acceleration of electronic structure calculations and for the development of linear-scaling algorithms will be discussed.

1Supported by NSF OCI 0749219 and DOE-SciDAC DE-FC02-06ER25794

4:30PM T13.00011 Improvements to the NRL Tight-Binding Model, MICHAEL MEHL, Naval Research Laboratory, DIMITRIS PAPACONSTANTOPOULOS, George Mason University, NOAM BERNSTEIN, Naval Research Laboratory, DANIEL FINKENSTADT, United States Naval Academy, STEFANO CURTAROLO, Duke University — The original NRL Tight-Binding Method[1] has proven to be extremely successful in reproducing first-principles total energies and band structures for many elemental systems[2], and has been applied in computationally intensive molecular dynamics simulations[3]. When generalizing to multiple atom types, however, some difficulties arise because of the form of the interaction of the on-site matrix elements with the external environment. We discuss these difficulties, and describe a new version of the method which includes a proper two-center development of the on-site parameters[4,5], including applications of the method. [1] RE Cohen et al., Phys. Rev. B 50, 14694 (1994) [2] MJ Mehl and DA Papanastasiou, Phys. Rev. B 54, 4519 (1996) [3] D Fin et al. and the gap energy and the gap between the conduction and the valence levels. This work was supported by the US Office of Naval Research. MJM is at Duke University under the NRL Advanced Graduate Research Program.
The Free energy of the landscape is calculated using these tiles and we discuss the role of these tiles in the liquid to liquid transition. The complete jamming local jamming structures to construct globally jammed states. We discuss the role of these tiles in the thermodynamic behavior of the corresponding liquid.
2:54PM T14.00003 Influence of Flow Quench Rate on the Internal Stress and Aging Dynamics of a Repulsive Colloidal Glass 1

Chinedum Osuji, Ajay Singh Negi, Department of Chemical Engineering, Yale University — We investigate the dynamics of aging in a repulsive colloidal glass composed of charged clay particles in aqueous suspension. Dynamic rheological measurements show a power law evolution of the elastic modulus of the system with sample age, measured as time elapsed after the cessation of a rejuvenating shear flow. We show that the scaling exponent is dependent on the rate of flow cessation or the flow quench rate. Comparatively fast quenches lead to systems with a smaller elastic modulus and accelerated aging whereas slower quenches result in higher modulus but correspondingly less rapid aging. We apply a recently proposed technique to follow the dynamics of residual or internal elastic stresses immediately after the flow arrest and find striking parallels between the relaxation of these stresses and the aging of the system. These results indicate that the evolution of the slow dynamics is strongly coupled to the internal stress state of the system and point to the identification of the flow quench rate as a mechanical variable that characterizes the system’s departure from equilibrium.

1 NSF CBET-0829005

3:06PM T14.00004 Hydrogen-bond network dynamics in sugar-based glasses, Marcus Cicerone, Jeraldine Johnson, NIST, Michael Pikal, University of Connecticut — Hydrophilic organic glasses composed of sugars and polysaccharides are known to stabilize proteins against aggregation and chemical degradation. It has long been supposed that, due to the long timescales involved in protein aggregation and chemical degradation in the glass, α relaxation processes essentially control the rate of degradation. We have shown that, although there may be > 7 orders of magnitude in time separation, β relaxation processes can dominate in influencing both chemical and physical degradation. Also, it is apparent that these β processes are closely related to dynamics of the hydrogen-bond network in these glasses. In this presentation we will briefly discuss the phenomenology of protein degradation in sugar-based glasses, and also present details of work on developing a fluorescent probe for use as a sensor for dynamics of the hydrogen-bond network in these glasses.

3:18PM T14.00005 Density of states and soft modes of hard sphere colloidal glasses — experimental observations, 1 Antina Ghosh, Vijayakumar Chikkadi, Peter Schall, University of Amsterdam, The Netherlands, Jorge Kurchan, ESPCI, France, Daniel Bonn, University of Amsterdam, The Netherlands — Recent theories and simulations have predicted the presence of soft modes due to which the DOS of glassy materials does not go to zero at zero frequency. We obtain DOS of colloidal hard sphere suspensions from experimental data. The displacement fields of hard sphere colloidal suspensions were studied for a range of volume fractions near the glass transition using confocal microscopy. Normal mode frequencies are then computed from the time averaged correlation matrix. The density of vibrational states obtained from normal mode analysis indeed reveals an excess of low frequency anomalous modes in the system. To understand the nature of the modes we analyse the displacement vector fields at various frequencies.

1 We acknowledge support from FOM and NWO.

3:30PM T14.00006 XPCS Studies of Nanoparticle Motion within Glassy Polymer Melts, H. Guo, JHU, G. Bourret, R. B. Lennox, M. Sutton, McGill U., J. L. Hardon, U. of Ottawa, R. L. Leheny, JHU — We report x-ray photon correlation spectroscopy (XPCS) experiments to investigate the motion of nanoscale gold particles within polyisobutene (PS) melts of molecular weight between 2K and 48K g/mol. The particles, with radius of approximately 2 nm, are dispersed in a highly dilute concentration (volume fraction 0.0004) and are functionalized with PS chains to stabilize them against aggregation. At high temperature, the observed motion is diffusive, with a rate that follows a Vogel-Fulcher temperature dependence. When the melts are quenched to lower temperature, the XPCS results indicate hyper-diffusive motion that can be modeled as strain in the melt in response to localized stress relaxation. These dynamics evolve with time following the quench, suggesting that they are coupled to aging of the polymer. Our observation of this hyper-diffusive motion among such a dilute concentration of stable nanoparticles indicates that the particles act as passive tracers and the motion is an intrinsic property of quenched melts.

3:42PM T14.00007 Divergent four-point dynamic density correlation function of a glassy suspension, 1 Grzegorz Szamel, Elijah Flennner, Department of Chemistry, Colorado State University — We use a diagrammatic formulation of the dynamics of interacting Brownian particles to study a four-point dynamic density correlation function of a glassy colloidal suspension. We re-sum a class of diagrams which separate into two disconnected components upon cutting a single propagator. The resulting formula for the four-point correlation function can be expressed in terms of three-point functions closely related to the three-point susceptibility introduced by Biroli et al. and the standard two-point correlation function. We numerically evaluate the four-point function and the associated dynamic correlation length. Both the amplitude of the four-point function and the correlation length diverge at the mode-coupling transition.

1 We acknowledge the support of NSF Grant No. CHE 0517709.

3:54PM T14.00008 Self-Organized Criticality in Periodically-Sheared Sedimenting Suspensions, EmmaNoEla Filippidi, Center for Soft Matter Research, New York University, Laurent Corre, Centre des Matériaux Mines, Paris, France, Paul Chakraborty, Center for Soft Matter Research, New York University — Suspensions of non-colloidal particles under slow periodic strain can undergo a dynamical phase transition from an active fluctuating state to an absorbing steady state at a critical volume fraction. In the case of density-mismatched particles, sedimentation and shear-induced diffusion drive the system towards a self-organized critical state. The lengthscales and timescales associated with the dynamics of the active particle clusters sustained near the critical point are shown to follow power-law behavior via simulation of activated random walkers. Finite-size effects and excluded volume interactions are explored for sedimenting and neutrally buoyant, mono- and bi-disperse suspensions both by simulation and experiment.

4:06PM T14.00009 Heat transfer in model amorphous solids, 1 Vincenzo Vitelli, Ning Xu, Department of Physics, University of Pennsylvania, Matthieu Wyart, HSEAS, Harvard University, Andrea Liu, Department of Physics, University of Pennsylvania, Sidney Nagel, James Frank Institute, University of Chicago — We investigate heat transfer in model amorphous solids obtained from jammed packings of soft spheres. At the boson peak frequency, we find a sharp crossover from a weak-scattering regime, in which the energy diffusivity drops rapidly with frequency, to a strong-scattering regime, in which the diffusivity is nearly frequency-independent. We present a scaling analysis of how the crossover frequency shifts to zero as the system is decompresed towards the jamming transition. We show that the regime of flat diffusivity, invoked to explain the temperature dependence of the thermal conductivity of glasses, can arise from properties of the jamming transition.

1 This work was supported by DE-FG02-05ER46199 (AJL, NX and VV), DE-FG02-03ER46088 (SRN and NX), NSF-DMR05-47230 (VV), and NSF-DMR-0213745 (SRN).
4:18PM T14.00010 Structural response of a colloidal glass to local forcing1, KEVIN B. APTOWICZ, West Chester University, PETER J. YUNKER, University of Pennsylvania, SEAN GOSSIN, West Chester University, ZEXIN ZHANG, A. G. YODH, University of Pennsylvania — Video microscopy of glassy colloidal suspensions permits direct visualization of particle locations and trajectories, thereby providing an excellent experimental tool to aid our understanding of glasses and address current theory. We have conducted a series of experiments utilizing a bidisperse mixture of thermosensitive NIPA microgel spheres to study the structural response of a two-dimensional colloidal glass to point expansion. The packing fraction of the colloidal suspension is tuned from a liquid to a deeply jammed glass by varying the global temperature of the sample. Over this range of packing fractions, the response of the sample to point expansion is analyzed. In particular, an infrared laser tightly focused on the sample generates thermophoretic forces that lead to a point expansion in the colloidal glass. We track particle rearrangements and characterize the response as a function of packing fraction. These experiments take a step towards understanding the relationship between local structure and bulk properties of glass.

3This research is supported by MRSEC grant DMR-0520020 (AGY), NSF grant DMR-080488 (AGY) and an award from Research Corporation (KBA).

4:30PM T14.00011 Relaxation processes in polystyrene melts and ultra-thin films . A. BALJON, S. WILLIAMS, San Diego State University, N. BALABAEV, Institute of Mathematical Problems of Biology, Pushchino, Russia, F. PAANS, A. LYULIN, Dutch Polymer Institute, Technical University Eindhoven, The Netherlands — By means of large-scale computer simulations we investigate relaxation processes in polystyrene melts and ultra-thin films. The local orientational mobility of the phenyl bonds is studied with the help of Legendre polynomials of the second-order P_2(t). The spectral density of P_2(t) shows several distinctive peaks. They are caused by the large-scale motions of cooperative segments (α relaxation), smaller-scale structural dynamics (β relaxation), and transient processes. Our simulations reveal that interfaces affect α- and β-relaxation processes differently. The most puzzling observation is a slight decrease in the structural relaxation time in the middle of the film, compared to that near the free surface. As expected, the connect non-nearest-neighbor sites. Free lattices exhibit highly anisotropic modes at k′ = 0, among which are soft modes with one-dimensional dispersion in wavenumber, giving rise to a flat density of states as a function of frequency ω. In the square lattice, these modes are shear acoustic phonons, whereas in the Kagome lattice, they are optical phonons. When k′ > 0, the low-energy modes cross over from acoustic phonons of the appropriate lattice symmetry for ω < ω∗ to the soft isostatic-like modes for ω > ω∗, and the density of states crosses over from Debye-like to flat. Static phonon response functions exhibit correlation lengths ξ ∼ 1/√R. We discuss the relation of these results to those for jammed systems near point J.

3MRSEC grant DMR-0520020 and NSF grant DMR-080488 (AGY) helped support this research.

4:42PM T14.00012 Changes in Local Structure and Dynamic Heterogeneity in an Aging Glass1, PETER YUNKER, ZEXIN ZHANG, University of Pennsylvania, KEVIN B. APTOWICZ, West Chester University, AHMED M. ALSAYED, CNRS/Rhodia, ARJUN YODH, University of Pennsylvania — Recent works have shown a connection between structure and dynamical heterogeneity in glass12. However, a connection between structure and aging dynamics remains elusive. To this end, we study aging in a bidisperse suspension of soft spheres. Micron-sized temperature-sensitive NIPA particles are employed in two-dimensions, and directly observed with video microscopy. After quenching from liquid to glass, the fraction of particles with crystalline order within the first coordination shell increases with time. Particles that undergo irreversible rearrangements exhibit correlation lengths that scale as the density of additional random bonds ∆. The real and imaginary part of the effective random-bond spring constants become 

5:06PM T14.00014 Periodic Lattices Near Isostaticity. ANTON SOUSLOV, T.C. LUBENSKY, Dept. of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — Lattices in d dimensions with with an average of z = 2d contacts per site are at the verge of mechanical stability and are called isostatic. Common isostatic latticess include the two-dimensional square and Kagome lattices as well as the three-dimensional cubic lattice with nearest-neighbor sites connected by central-force springs of spring constant k and randomly packed spheres at random close packing at what is called point J. We calculate the phonon response functions and spectra of nearly isostatic square, cubic, and Kagome lattices in which springs of spring constant k′ connect next-nearest-neighbor sites. These lattices exhibit highly anisotropic modes at k′ = 0, among which are soft modes with one-dimensional dispersion in wavenumber, giving rise to a flat density of states as a function of frequency ω. In the square lattice, these modes are shear acoustic phonons, whereas in the Kagome lattice, they are optical phonons. When k′ > 0, the low-energy modes cross over from acoustic phonons of the appropriate lattice symmetry for ω < ω∗ to the soft isostatic-like modes for ω > ω∗, and the density of states crosses over from Debye-like to flat. Static phonon response functions exhibit correlation lengths ξ ∼ 1/√R. We discuss the relation of these results to those for jammed systems near point J.

4:54PM T14.00013 Investigation of electron beam induced changes in glassy Ge_xSe_1-x thin films1 . W. ZHOU, G. HOFFMAN, H.O. COLIJN, R.M. REANO, R. SOORYAKUMAR, The Ohio State University, P. BOOLCHAND, University of Cincinnati — Global structures in network glasses are characterized by their connectedness or mean co-ordination number. As the number of these cross-links within a covalent network increases by compositional tuning these systems steadily evolve from being underconstrained (floppy) to an overconstrained (rigid) solid. Recently (Appl Phys Lett 93, 041107 (2008)) we exploited electron beams to write nanoscale surface motifs in Ge_xSe_1-x thin films that are at the special Ge in Se composition lying in the immediate vicinity of the floppy to rigid stiffness transition. In order to investigate the nature of the surface reliefs we have employed selected area transmission electron microscopy (STEM) to probe the electron beam induced structural changes to the film. Films of thicknesses less than 150 nm were deposited by pulsed laser deposition directly onto a carbon film on a mica substrate. The glass film and carbon layer were then lifted off onto copper grids for the TEM studies. Extension of the electron beam driven studies to other compositions, as well as the effect of multiple beam overwrites on the surface reliefs and trenches in several Ge_xSe_1-x compositions will also be presented.

1Supported by NSF through Grant No. ECCS 0701686.

5:06PM T14.00014 Periodic Lattices Near Isostaticity . ANTON SOUSLOV, T.C. LUBENSKY, Dept. of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA 19104 — Lattices in d dimensions with with an average of z = 2d contacts per site are at the verge of mechanical stability and are called isostatic. Common isostatic latticess include the two-dimensional square and Kagome lattices as well as the three-dimensional cubic lattice with nearest-neighbor sites connected by central-force springs of spring constant k and randomly packed spheres at random close packing at what is called point J. We calculate the phonon response functions and spectra of nearly isostatic square, cubic, and Kagome lattices in which springs of spring constant k′ connect next-nearest-neighbor sites. These lattices exhibit highly anisotropic modes at k′ = 0, among which are soft modes with one-dimensional dispersion in wavenumber, giving rise to a flat density of states as a function of frequency ω. In the square lattice, these modes are shear acoustic phonons, whereas in the Kagome lattice, they are optical phonons. When k′ > 0, the low-energy modes cross over from acoustic phonons of the appropriate lattice symmetry for ω < ω∗ to the soft isostatic-like modes for ω > ω∗, and the density of states crosses over from Debye-like to flat. Static phonon response functions exhibit correlation lengths ξ ∼ 1/√R. We discuss the relation of these results to those for jammed systems near point J.

5:18PM T14.00015 Soft modes and elasticity of nearly isostatic lattices: randomness and dissipation1 . XIAOMING MAO, TOM LUBENSKY, Department of Physics and Astronomy, University of Pennsylvania — Isostatic periodic lattices, such as the square and Kagome lattices in spatial dimension d = 2, are systems at the onset of rigidity. They are marginally stable with coordination number z = 2d, and they may exhibit a non-extensive number of soft modes that can be removed by adding an infinitesimal number of additional bonds. Randomly packed frictionless spheres at the jamming point J represent an important isostatic system that, because of its randomness, exhibits complexities beyond those of periodic systems. To study the effects of randomness on phonon response, propagation, and damping, we constructed model lattices near isostaticity by adding randomly distributed next-nearest and second-nearest neighbor bonds to the isostatic square and Kagome lattices, respectively. We calculated a number of properties of these models using the CPA approximation and found them to resemble those of jammed solids near the point J. In particular, the phonon density of states crosses over from Debye-like at low frequency ω to the flat frequency-independent behavior of a one-dimensional systems at a characteristic frequency ω∗ that scales as the density of additional random bonds Δz. The real and imaginary part of the effective random-bond spring constants become equal at ω∗. We also identify a characteristic length that scales as (Δz)^-1.

1This work was supported by NSF under grant No. DMR 0804900.
2:30PM T15.00001 Time evolution of distributive entropy in rectangular microchannel mixers, MIRON KAUFMAN, PETRU FODOR, Cleveland State University — Patterning ridges on the surface of microchannels has been found to be a viable strategy to induce mixing in straight channels, despite the characteristically small Reynolds numbers. In this work we evaluate the time evolution of the Rényi entropy associated with the spatial distribution of tracers advected by an incompressible fluid moving in several straight rectangular channels: staggered herring bone [1], fractal surface patterning [2]. The steady state flow fields are obtained by solving the Navier–Stokes and continuity equations using a finite element analysis package. The Rényi entropy is then evaluated at different times using the spatial distribution of the tracers. The entropy increases with time as Int with a slope approximately equal to unity. The slope quantifies the rate of distributive mixing. The rate of increase in the entropy is found to be independent of the Rényi beta parameter. This is qualitatively different than the distributive mixing in channels with moving walls [3] where the rate of distributive mixing changes with the beta parameter. We also study the dependence of the distributive entropy on the Reynolds number. [1] A.D. Stroock et al., Science 295, 647 (2002); [2] M. Camesasca, M. Kaufman, I. Manas-Zloczower, J. Micromech. Microeng. 16, 2298 (2006); [3] W. Wang, I. Manas-Zloczower, M. Kaufman, Chemical Engineering Communications, 192(4), 405-423 (2005).

2:42PM T15.00002 Capillary absorption of metal nanodroplets by carbon nanotubes, SHAUN HENDY, Industrial Research Ltd, DMITRI SCHEBACHOV, Victoria University of Wellington — We present a simple model that demonstrates the possibility of capillary absorption of non-wetting liquid nanoparticles by carbon nanotubes assisted by the action of the Laplace pressure due to the droplet surface tension. We test this model with molecular dynamics simulation and find excellent agreement with the theory, which shows that for a given nanotube radius, there is a critical size below which a metal droplet will be absorbed. We then consider the dynamics of capillary absorption using the steady-state flow model due to Marmur, which is based on the Lucas-Washburn model with the addition of a driving force due to the Laplace pressure of the droplet. We find an exact solution to the absorption problem, which shows a logarithmic time dependence for a non-marmur’s limit. For Marmur’s limit the steady state is approached very slowly with time and shows that this reproduces the dynamics observed in the simulations well. The simulations show that the flow of the metal exhibits a large degree of slippage at the tube walls, with slip lengths of up to 10nm. These findings suggest new methods for fabricating composite metal-CNT materials, and have implications for our understanding of the growth of CNTs from metal catalyst particles. The results also explain the recent observations of the absorption of Cu nanodroplets by carbon nanotubes.

2:54PM T15.00003 Dynamic Pattern Formation In a Bubble-Generating Concentric Microfluidic Device1, KENG-HUI LIN, KUO-YUAN CHUNG, Institute of Physics, Academia Sinica, Taipei, Taiwan — We observe rich spatiotemporal patterns of bubbles inside liquid droplets through a concentric microfluidic device made by two capillary tubes flown with gas and liquid respectively. When the gas pressure increases, the bubbles change from monodisperse, bidisperse to polydispers. When the liquid flow rate to the gas flow rate is small, the bubble can not be stabilized inside the liquid droplet. The diameter of the bubbles can be scaled with the ratio of gas flow rate to the liquid flow rate. Our device offers different geometry to understand the bubble breakup in the microfluidic device.

3:06PM T15.00004 Flow-Based Organization of Soft Matter in Three Dimensions, LIAN LENG, SIASHAS ASLANBEIGI, AXEL GUENTHER, University of Toronto — Flows of miscible and immiscible liquids through microchannel networks have been previously used to achieve spatial organization within one plane. However, extending this approach to three dimensions, an essential requirement to create synthetic bulk materials with a regular microstructure, is not straightforward. To our knowledge for the first time, we demonstrate microfluidic strategy for the three-dimensional organization of soft bulk materials. The approach is enabled by a massively scaled microfluidic architecture that distributes two miscible or immiscible fluid streams through an array of parallel channels. The soft-lithographic fabrication process was adapted to consistently define microfluidic channel networks in elastomer substrates that are only 500 microns thin; followed by subsequent bonding of up to ten such layers in the vertical direction. The chip was connected with fluidic inlets, completely immersed in water and continuously extruded the organized material at its exit. Upon leaving the chip, neighbouring fluid streams from each level are allowed to separate naturally. The material microstructure was controlled by adjusting the flow rates of the interdiffusing fluid streams (e.g. aqueous alginate and calcium chloride solutions).

3:18PM T15.00005 Viscous droplet deformation and breakup in microfluidic cross-flows, THOMAS CUBAUD, Stony Brook University — The dynamic response of translating high-viscosity droplets is experimentally investigated by means of a sharp increase of the flow velocity in a microchannel junction. The additional local injection of the continuous phase from symmetric side-channels into a square microchannel produces a broad range of time-dependent deformations and breakup. In particular, due to microscale wall confinement, the system displays a non-linear behavior with the initial droplet size. Deformations, relaxation times, and fragmentation processes are examined as a function of flow and fluids properties with a particular emphasis on the formation of slender viscous structures and spoon-like droplets, i.e., asymmetrical droplets.

3:30PM T15.00006 Morphology of liquids spreading along open nanofluidic channels1, ANTONIO CHECCO, Brookhaven National Laboratory — Dynamic atomic force microscopy (AFM) in the non-contace regime is used to study the morphology of a non-volatile liquid (squalane) as it spreads along wettable nanostripes embedded in a non-wettable surface. AFM allows the direct observation of the microscopic contact line of spreading nanoliquids with unprecedented spatial resolution. Results show that the liquid profile depends on the amount of lateral confinement imposed by the nanostripes and it is truncated at the microscopic contact line in good qualitative agreement with classical mesoscale hydrodynamics. However, the width of the contact line is found to be significantly larger than expected theoretically. This behavior may originate from small chemical inhomogeneity of the patterned stripes as well as from thermal fluctuations of the contact line.

3:42PM T15.00007 Separation of chiral objects by shear flow in microfluidic channels - Theory, HENRY FU, Brown University, MARCOS, MIT, THOMAS POWERS, Brown University, ROMAN STOCKER, MIT — Motivated by the desire to separate chiral molecules, we investigate the motion of helices in shear flow generated by a microfluidic channel. We present a model based on resistive force theory to show that hydrodynamic forces on a helix in shear flow produce a drift perpendicular to the shear plane. The drift depends on the sign of the shear rate and the chirality of the helix. Net drift results from preferential alignment with streamlines. For large (>1 micron), elongated particles, alignment is a consequence of the deterministic tumbling trajectories (Jeffery orbits) in shear flow. For smaller particles, we estimate the effect of Brownian rotational diffusion on chirality-sensitive drift. We deduce a lower size limit for separation of chiral objects by shear flow in microfluidic channels.
Separation of chiral objects by shear flow in microfluidic channels - Experiment.
Marcos, Massachusetts Institute of Technology, Henry Fu, Thomas Powers, Brown University, Roman Stocker, Massachusetts Institute of Technology — We use microfluidics to test the prediction that a helix in shear flow drifts across streamlines. We use the non-motile, helical-shaped bacterium Leptospira biflexa as our model chiral object. As the shear in the top and bottom halves of the microchannel has opposite sign, we predict and observe the bacteria in these two regions to drift in opposite directions. The magnitude of the separation is in good agreement with theory.

Tunable liquid optics: electrowetting-controlled liquid mirrors based on self-assembled Janus tiles.
Tom Krupenkin, University of Wisconsin – Madison, Mike Bucaro, Harvard University, Paul Kolodner, Bell Laboratories, Ashley Taylor, University of Wisconsin – Madison, Alex Sidorenko, University of the Sciences in Philadelphia, Joanna Aizenberg, Harvard University — In this work we describe a tunable, high-reflectivity optofluidic device based on self-assembly of anisotropically-functionalized hexagonal micromirrors (Janus tiles) on the surface of an oil droplet to create a concave liquid mirror. The liquid mirror is deposited on a patterned transparent electrode that allows the focal length and axial position to be electronically controlled. The mirror is mechanically robust and retains its integrity even at high levels of vibrational excitation of the interface. The use of reflection instead of refraction overcomes the limited available refractive-index contrast between pairs of density-matched liquids, allowing stronger focusing than is possible for a liquid lens of the same geometry. This approach is compatible with optical tools that could provide novel functionality — for example, a dynamic 3D projector; i.e., a light source which can scan an image onto a moving, non-planar focal surface. Janus tiles with complex optical properties can be manufactured using our approach, thus potentially enabling a wide range of novel optical elements.

Designing actuated cilia pumping fluids in microchannels.
Alex Alexeev, Georgia Institute of Technology, Julia Yeomans, University of Oxford, Anna C. Balazs, University of Pittsburgh — Using three-dimensional computational modeling, we examine the motion of actuated cilia in a fluid-filled microchannel. The cilia are modeled as deformable, elastic filaments, which are initially tilted with respect to the channel surface. A sinusoidal force normal to the microchannel wall is applied at the free ends of the tilted cilia and induces periodic oscillations of these flexible filaments. To capture the complex fluid-structure interactions among these filaments, the channel walls and the surrounding solution, we employ our hybrid computational approach that combines a lattice Boltzmann model for hydrodynamics of viscous fluids and a lattice spring model for the micromechanics of elastic solids. We find that the actuated cilia give rise to a unidirectional flow in the microchannel and by simply altering the frequency of the applied force, we can controllably switch the direction of the net flow. The findings suggest that beating elastic cilia could be harnessed to regulate the fluid streams in microfluidic devices.

A Deterministic Microfluidic Ratchet.
Kevin Louterback, Jason Puchalla, Robert Austin, James Sturm, Princeton University — We present a deterministic microfluidic ratchet where the trajectory of particles in a certain size range is not reversed when the sign of the driving force is reversed. This ratcheting effect is produced by employing triangular rather than the conventionally circular posts. When the sign of the driving force is reversed, the particles may bounce together and merge into one when triggered with electric fields that are created by the chip. [1] TP Hunt, D Issadore, RM Westervelt – Lab on a Chip, 2008.

Topological Dependence of ds-DNA Confined in Nanoslits.
Po-Keng Lin, Institute of Atomic and Molecular Science, Academia Sinica, Jen-Fang Chang, Institute of Physics, Academia Sinica, Cheng-Hung Wei, Pei-Kuen Wei, Research Center for Applied Sciences, Academia Sinica, Y.-L. Chen, Institute of Physics, Academia Sinica — Topological constraints are important for the DNA condensation in confinement, such as chromosome in the cell and bacteriophage DNA packaging. We investigated the topological dependence of the size, shape and diffusivity of ds-DNA confined in a nanowire with height \(h = 780 \text{ nm}\) (< bulk radius of gyration of ds-DNA) to strong confinement \(h = 20 \text{ nm} < \kappa\) persistence length \(\lambda_p\) are systematically investigated. Shape anisotropy of both linear and circular DNA increases with decreasing \(h\), which indicate the DNA become more anisotropic. Furthermore, we observed the transition from de Gennes to Odijk scaling in the measured extension and diffusivity when \(h = \kappa\lambda_p\). Interestingly, the diffusivity of circular DNA is larger than linear DNA in the birebodl regime, but they are nearly equal in slits with \(h << \kappa\lambda_p\).

Propagation modes of entropically trapped and extended DNA molecules.
Morten Mikkelsen, Technical University of Denmark, Walter Reisner, Brown University, Henrik Flyvbjerg, Anders Kristensen, Technical University of Denmark — Nanconfinement is a powerful tool for controlling polymer conformation and dynamics in lab-on-a-chip type devices for the analysis of DNA and other biomolecules. We present a new device that combines confinement-based extension of DNA with the entropic trapping principle, leading to qualitatively new physics and applications. The device consists of a 50 nm slit channel with an array of transverse \(100 \times 100\) nm grooves, where the transport of DNA molecules perpendicular to the groove axis is investigated under pressure driven buffer flow. At low flow velocities the DNA remains trapped and extended in the nanogrooves while buffer circulates through the slit, enabling physical mapping of the DNA while performing real time buffer exchanges. For flow velocities above a molecular weight dependent escape threshold, we show that the molecule transport through the slit channel randomly alternates between two modes of propagation: A stepwise groove to groove hopping, called the ‘sidewinder’, and a continuous tumbling across the grooves, where the molecules feel the topology as an effective friction, called the ‘tumbleweed’. The observed length dependence on the molecule velocity may lead to a novel separation methodology.

Multiplex selection and elution of aptamers using nanoporous sol-gel droplets and a microheater array.
Seung-Min Park, Cornell University, Jiyoung Ahn, MinJoung Jo, Soyun Kim, Donguk University, Dong-Ki Lee, Sungkyunkwan University, John LIs, Pangshun Zhu, Harold Craighead, Cornell University — Aptamers are well-known protein capture reagents that bind to specific proteins and can be effective in inhibiting the protein’s normal interactions. Here, we have described a process for selective binding and elution of aptamers from the nanoporous-silicate sol-gel droplets within which target proteins are immobilized. These silicate sol-gel droplets are incorporated with polydimethylsiloxane (PDMS) microfluidic systems and individually addressable by electrical microheaters. These properties allow discrete protein – nucleic acids interaction so that multiplexed selection is possible. It is shown that specific aptamers bind their respective protein targets and can be selectively eluted by micro-heating. Our microfluidic in vitro selection system improves selection efficiency, reducing the number of selection cycles needed to produce high affinity aptamers. We are also able to separate high-affinity nucleic acid species from a large random nucleic acid pool. The process is readily scalable to larger arrays of sol-gel-embedded proteins.
2:30PM T16.00001 Probing quasiparticle dispersion and order parameter symmetry of ultracold fermionic superfluids and density waves via lattice. DAVID PEKKER, RAJDEEP SENSARMA, EUGENE DEMLER, Harvard University. We propose a pump-probe experiment for studying the properties of condensed states of ultracold fermionic atoms in optical lattices. The pump consists of periodic modulations of the optical lattice potential in time, and the probe of measuring either the momentum distribution function or the density-density correlation functions. We apply our scheme to probing d-wave superfluids and d-density waves. In both cases we show that the dispersion relation of quasi-particles can be extracted from the momentum distribution function, and the order-parameter symmetry can be extracted from the pattern of peaks and dips that form due to the interference of the excited quasiparticles in the appropriate density-density correlation function.

2:42PM T16.00002 Relaxation of Double Occupancies in large U Hubbard Model. EUGENE DEMLER, RAJDEEP SENSARMA, DAVID PEKKER, Harvard University. We study the relaxation rates of double occupancies in large U Fermionic Hubbard model both in the Mott insulating state and in the compressible state with holes. We find that the relaxation rate \( \sim t \exp(-U/t) \) in the insulating state and \( \sim t \exp(-U/2t) \) in the compressible state.

2:54PM T16.00003 Modulation of Optical Lattice Potential in a Fermionic Mott Insulator. RAJDEEP SENSARMA, DAVID PEKKER, EUGENE DEMLER, Harvard University. We analyze the double occupancies produced in a Fermionic Mott insulator near half-filling by modulating the optical lattice potential. We relate the rate of production of doublons to the spectral function of a hole and a doublon in the background of the spins. In the high temperature (spin disordered) state, the hole (doublon) is completely incoherent and the rate of production of doublons is peaked around \( \omega = U \) and decreases monotonically up to twice the bandwidth on either side. We also derive a sum-rule for energy integrated response in this limit. At low temperatures (anti-ferromagnetically ordered state), the spin ordering leads to a coherent peak in the hole spectral function along with other broad features corresponding to shake-off of spin-waves. This shows up in the doublon production rate as a sharp edge at the lower end of the spectrum and oscillations as a function of perturbing frequency.

3:06PM T16.00004 Equation of state and magnetic properties of the three-dimensional repulsive Hubbard model. CHIA-CHEN CHANG, SHIWEI ZHANG, Department of Physics, The College of William and Mary. Motivated by recent advances in fermionic optical-lattice experiments, we report results from numerical simulations of the ground state properties of the three-dimensional single-band Hubbard model (with nearest-neighbor hopping and repulsive \( s \)-wave on-site interaction). We focus on intermediate interaction strengths, \( U/t < \sim 10 \). The constrained-path auxiliary-field quantum Monte Carlo method is used, with a phaseless approximation to control the sign/phase problem. One-body finite size effects and shell effects are eliminated by implementing twist-averaged boundary conditions. The equation of state is determined accurately for several values of \( U/t \). We study the nature of the ground state away from half-filling by examining the spin-spin and other correlation functions as a function of doping.

3:18PM T16.00005 Phase diagram and Neel temperature of fermions in a three-dimensional optical lattice. CHARLES MATHY, DAVID HUSE, Princeton University. One of the most exciting prospects in the field of ultracold atoms is the experimental realization of an antiferromagnetic Mott state, in a system of fermions in a three-dimensional optical lattice. Experimentalists are currently wrestling with achieving the requisite ordering temperatures. We address the question of which regions of parameter space one should explore to find the highest Neel temperature. To this end, we perform Hartree-Fock calculations and map out the magnetic phase diagram of two component fermions in a three-dimensional simple cubic lattice. We find that the superexchange and Neel temperature are maximized in a regime of intermediate coupling, where the system is no longer well described by a one-band Hubbard model. We also perform a perturbative expansion in a Wannier basis, and study the corrections to the Hubbard model in this region. We find that the largest correction is a Hund's rule ferromagnetic coupling. Finally, our calculations suggest that the Mott plateau should be large in the intermediate coupling regime, and therefore experimentally accessible.

3:30PM T16.00006 Collisional cooling of ultra-cold atom ensembles using Feshbach resonances. LUDWIC MATHEY, EITE TIESINGA, PAUL JULIENNE, CHARLES CLARK, NIST and JQI. We propose a new type of cooling mechanism for ultra-cold fermionic atom ensembles, which capitalizes on the energy dependence of inelastic collisions in the presence of a Feshbach resonance. We first discuss the case of a single magnetic resonance, and find that the final temperature and the cooling rate is limited by the width of the resonance. A concrete example, based on a \( p \)-wave resonance of \(^{40}\text{K}\), is given. We then improve upon this setup by using both a very sharp optical resonance and a very broad magnetic resonance and show that one can reach temperatures competitive to those created by current technologies.

3:42PM T16.00007 Fulde-Ferrell-Larkin-Ovchinnikov-like pairing of attractively interacting fermions on a two-leg ladder geometry. FABIAN HEIDRICH-MEISNER, RWTH Aachen University, ADRIAN FEIGUIN, Microsoft Q, UC Santa Barbara, and U of Maryland. Recent experiments on spin-imbalanced ultracold Fermi gases at MIT and Rice have stimulated an active search for conditions that would allow for the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state to be realized in ultracold atomic gases. Theoretical work indicates that FFLO-like pairing is favored in low-dimensions (see [1] and references therein). Indeed, in one-dimensional (1D) optical lattices, the FFLO pairing mechanism is a dominating feature and survives in the presence of a confining potential. Here we extend our previous study [1] to the case of a two-leg ladder geometry [2]. Experimentally, ladders can be realized as arrays of double wells. Using a numerically exact approach, the density matrix renormalization group method, we show that FFLO-like pairing is found in a large part of the respective phase diagram, with an order parameter with a much richer structure than in the strict 1D case. We further shed light on the effect of a harmonic potential as present in optical lattices and establish the emergence of two-dimensional physics and a novel phase separation scenario not encountered in 1D chains.


3:54PM T16.00008 Complete Phase Diagram of the Attractive Hubbard Model with a Zeeman Field. YEN LEE LOH, The Ohio State University, NANDINI TRIVEDI. We study the attractive Hubbard model on square and cubic lattices, using a variational mean-field theory in which the interaction is decoupled in six channels (spin, charge, and pairing). We present the phase diagram as a function of attraction U, chemical potential mu, and Zeeman (spin-exchange) field h, and also as a function of the numbers of up and down spins. We test our hypothesis that FFLO states have a larger range of stability in a lattice than in the continuum, especially in lower dimensions. We discuss the results in the context of ultracold fermions in optical lattices, as well as the implications for thin film superconductors in a parallel magnetic field.
4:06PM T16.00009 Orbital Analogue of the Quantum Anomalous Hall Effect in p-Band cold fermion Systems. CONGJUN WU, Department of Physics, UCSD — We investigate the topological insulating states of the p-band systems in optical lattices induced by the on site orbital angular momentum polarization, which exhibit gapless edge modes in the absence of Landau levels. This effect arises from the energy-level splitting between the on site px,py and px-ipy orbitals by rotating each optical lattice site around its own center. At large rotation angular velocities, this model naturally reduces to two copies of Haldane’s quantum Hall model. The distribution of the Berry curvature in momentum space and the quantized Chern numbers are calculated. The experimental realization of this state is feasible.

4:18PM T16.00010 Anomalous expansion of attractively interacting Fermions in an optical lattice. TAKUYA KITAGAWA, Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA, LUCIA HACKERMULLER, ULRICH SCHNEIDER, MARIA MORENO-CARDONER, THORSTEN BEST, SEBASTIAN WILL, Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany, EUGENE DEMLER, Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA, IMMANUEL BLOCH, BELEN PAREDES, Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, D-55099 Mainz, Germany — We consider a two component Fermi mixture of ultracold atoms with attractive interactions in an optical lattice and in the presence of a parabolic potential. Using a high temperature expansion, we analyze the behavior of the system size when adiabatically increasing the interaction strength. We show that entropy conservation leads to an anomalous radius increase for large values of the interaction. We also find that the competition between entropy and the Hartree part of the attractive interaction makes the system reach a minimum size at a nonzero value of the interaction.

1Harvard-MIT CUA, DARPA, MURI, and the NSF

4:30PM T16.00011 Strongly correlated Fermions in optical lattices: static and dynamic properties. LUCIA HACKERMULLER, ULRICH SCHNEIDER, MARIA MORENO-CARDONER, Johannes-Gutenberg-University Mainz, Germany, IMMANUEL BLOCH, Universität Mainz, Max Planck Institut für Quantenoptik, Garching, Germany — Fermionic atoms in optical lattices can serve as a model system for condensed matter physics. They implement the Hubbard model with high experimental control of the relevant parameters. We study static and dynamic properties of ultracold fermions in different regimes, varying from a metal to a band insulator in the non-interacting system and including complex metals and the Fermionic Mott Insulator for strongly repulsive systems. In the experiment, spin mixtures of fermionic 40K are loaded into a combination of a blue detuned three dimensional optical lattice and a red detuned dipole trap. This combination of optical potentials allows an independent control of lattice depth and harmonic confinement, thus enabling us to explore different regimes. In addition to the static properties we present measurements of the dynamic response of the system to changes of the external parameters.

4:42PM T16.00012 Attractively Interacting Fermions in an Optical Lattice. LUCIA HACKERMULLER, ULRICH SCHNEIDER, MARIA MORENO-CARDONER, Johannes-Gutenberg-University Mainz, Germany, TAKUYA KITAGAWA, Department of Physics, Harvard University, THORSTEN BEST, SEBASTIAN WILL, SIMON BRAUN, Johannes-Gutenberg-University Mainz, Germany, EUGENE DEMLER, Department of Physics, Harvard University, BELEN PAREDES, IMMANUEL BLOCH, Johannes-Gutenberg-University Mainz, Germany — Mixtures of ultracold fermionic species in optical lattices can serve as a tool to test condensed matter physics models, a prominent example being the Fermi-Hubbard-Hamiltonian. We study a balanced spin mixture of 40K in |F,m_F⟩ = (1/2, 1/2) and (3/2, 7/2) in a three dimensional blue detuned optical lattice, where the interaction between the spin states can be tuned via a Feshbach resonance. Changing the scattering length allows us to go from non-interacting to attractive states and finally to a strongly paired system. For small attractive interactions, the cloud size shrinks upon increasing the interactions, but surprisingly we find a minimal cloud size for medium attractive interactions. For stronger interactions the cloud size increases again. This anomalous increase can be understood with a straightforward entropy argument. We compare the experimental data with the prediction of an exact calculation in the two-tunneling limit and with a high temperature expansion theory.

4:54PM T16.00013 Spin and Charge Dynamics in Atomic Fermions Loaded on Optical Lattice. MASAHIKO OKUMURA1, CCSE, Japan Atomic Energy Agency, HIROAKI ONISHI, Advanced Science Research Center, Japan Atomic Energy Agency, SUSUMU YAMADA2, MASAHIKO MACHIDA2, CCSE, Japan Atomic Energy Agency — We study spin and charge dynamics of trapped two-component fermions loaded on an optical lattice by using the time dependent density matrix renormalization group (TDDMRG) method. The present target issue is dynamics of spin and charge in Mott state recently realized experimentally by [1]. Firstly, we simply shake a trapped potential superposed onto an optical lattice and observe the charge dynamics on the Mott state by using TDDMRG. Secondly, we do the same thing on a trapped potential which works only on a pseudo-spin species and observe the spin density dynamics. These results are compared with non-trapped case with an open boundary condition. Also, we compare one-dimensional chain like cases with those of n-legs square and triangular ladder systems. References [1] U. Schneider, L. Hackermuller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, A. Rosch, arXiv:0809.1464.

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5:06PM T16.00014 ABSTRACT WITHDRAWN —

5:18PM T16.00015 Multiband superfluidity and superfluid-insulator transition of strongly interacting fermions in an optical lattice. ANTON BURKOV, University of Waterloo, ARUN PARAMEKANTI, University of Toronto — We study the multiband superfluid phase and superfluid-insulator transition of strongly interacting fermionic cold atoms in an optical lattice at a filling of two fermions per lattice site. Our mean-field approach includes both Hartree and pairing correlations and thus differs from previous approaches to this problem. We point out a very significant discrepancy between the mean-field theory result for the critical lattice depth of the superfluid-insulator transition and its experimental value. We show that this discrepancy is due to a very small superfluid stiffness of the paired fermion superfluid in a deep optical lattice. We also present new experimentally testable results on the modulated components of the superfluid order parameter, quasiparticle gap, and band occupation as a function of the lattice depth.

Wednesday, March 18, 2009 2:30PM - 5:30PM —
Session T17 GQI: Focus Session: Materials in Superconducting Qubits 318
2:30PM T17.00001 Noise and Dephasing from Surface Magnetic States in Superconducting Circuits. ROBERT MCDERMOTT, University of Wisconsin — Superconducting qubits are a leading candidate for scalable quantum information processing. In order to realize the full potential of these qubits, it is necessary to develop a more complete understanding of the microscopic physics that governs dissipation and dephasing of the quantum state. In the case of the Josephson phase and flux qubits, the dominant dephasing mechanism is an apparent low-frequency magnetic flux noise with a 1/f spectrum and a magnitude of several μΦ0/Hz1/2 at 1 Hz, where Φ0 = h/2e is the magnetic flux quantum. Recent qubit results are compatible with the excess low-frequency noise measured by researchers at Berkeley more that 20 years ago in a series of experiments on SQUIDs cooled to millikelvin temperatures. The origin of this excess noise was never understood. Here we describe studies of flux noise and temperature-dependent magnetization in SQUIDs cooled to millikelvin temperatures. We observe that the flux threading the SQUIDs increases as 1/T as temperature is lowered; moreover, the flux change is proportional to the density of trapped vortices. The data is compatible with the thermal polarization of unpaired surface spins in the trapped fields of the vortices. In the absence of trapped flux, we observe evidence of spin- glass freezing at low temperature. These results suggest a microscopic explanation for the universal 1/f flux noise in SQUIDs and superconducting qubits, and suggest that suitable surface treatments of the superconducting films will lower the density of magnetic states, leading to superconducting devices with lower noise and solid-state qubits with improved coherence times.

3:06PM T17.00002 Susceptibility of Magnetic Surface States in Superconducting Circuits. STEVEN SENDLEBACH, DAVID HOVER, ROBERT MCDERMOTT, UW-Madison Department of Physics, MICHAEL MUECK, Institut für Angewandte Physik, Justus-Liebig-Universität, Gießen — Recent experiments indicate that there is a high density of unpaired spins residing on the surfaces of superconducting thin films used to implement SQUIDs and superconducting qubits. Fluctuations of these spins give rise to low frequency flux noise and dephasing of the qubit state. Realization of phase and flux qubits with improved dephasing times will require a deeper understanding of the microscopic physics that governs fluctuations of the surface spins. Here we describe experiments that probe the ac spin susceptibility of the surface magnetic states. The detector is a dc SQUID-based susceptometer optimized for the study of surface spins. We discuss the temperature and frequency dependence of the spin susceptibility, and relate these to interactions between spins, the distribution of spin relaxation times, and possible spin-glass freezing.

3:18PM T17.00003 Reflectometry measurements of 1/f noise in SQUID phase qubits at mK temperatures1. B. K. COOPER, R. M. LEWIS, CNAM and JQI, University of Maryland, B. S. PALMER, V. ZARETSKEY, Laboratory for Physical Sciences, A. J. PRZYBYSZ, H. KWON, J. R. ANDERSON, C. J. LOBB, F. C. WELLSTOOD, CNAM and JQI, University of Maryland — We measure 1/f noise spectra in dc SQUID phase qubits using a microwave reflectometry technique. One of the SQUID junctions is shunted by a large capacitor, forming a microwave frequency resonator biased and driven to show nonlinear response, typically at 1.5 GHz. This nonlinearity means small current or flux fluctuations produce large changes in reflected phase which we can measure using homodyne detection. Measurements from aluminum qubits on sapphire are compared to previous measurements of 1/f noise flux in SQUIDs and a similarly designed Nb/AIOx/Nb on silicon dc SQUID fabricated by Hynes; data was taken at temperatures ranging from 50 mK to 500 mK. 1This work was supported by JQI, CNAM and LPS.

3:30PM T17.00004 Crystalline Silicon Dielectrics for Superconducting Qubit Circuits. DAVID HOVER, WEINA PENG, STEVEN SENDLEBACH, MARK ERIKSSON, ROBERT MCDERMOTT, University of Wisconsin Madison — Superconducting qubit energy relaxation times are limited by microwave loss induced by a continuum of two-level state (TLS) defects in the dielectric material of the circuit. State-of-the-art phase qubit circuits employ a micron-scale Josephson junction shunted by an external capacitor. In this case, the qubit T1 time is directly proportional to the quality factor (Q) of the capacitor dielectric. The amorphous capacitor dielectrics that have been used to date display intrinsic Q of order 1010 to 1011. Shunt capacitors with a Q of 103 are required to extend qubit T1 times well into the microsecond range. Crystalline dielectric materials are an attractive candidate for qubit capacitor dielectrics, due to the extremely low density of TLS defects. However, the robust integration of crystalline dielectrics with superconducting qubit circuits remains a challenge. Here we describe a novel approach to the realization of high-Q crystalline capacitor dielectrics for superconducting qubit circuits. The capacitor dielectric is a crystalline silicon nanomembrane. We discuss characterization of crystalline silicon capacitors with low-power microwave transport measurements at millikelvin temperatures. In addition, we report progress on integrating the crystalline capacitor process with Josephson qubit fabrication.

3:42PM T17.00005 Testing of qubit materials and fabrication using superconducting resonators. SHWETANK, KUMAR, MATTHIAS STEFFEN, DAVID DIVINCENZO, GEORGE KEEFE, MARY BETH ROTHWELL, MATTHEW FARINELLI, JIM ROZEN, FRANK MILLIKEN, MARK KETCHEN, IBM Research — We will present the results of measuring a superconducting resonator fabricated using different substrates and superconducting metals. Specifically, the quality factor of these resonators will be shown to be closely related to not only the purity of the substrates and metals used in the process but also to the details of the fabrication. We will demonstrate the change in quality factor of a bare resonator when subjected to the qubit process. Based on our measurements we propose that superconducting resonators may form a test bed for troubleshooting the fabrication process for minimizing the materials related dissipation in the qubits.

3:54PM T17.00006 Optimizing silicon nitride for superconducting quantum circuits. HANHEE PAIK, KEVIN OSBORN, Laboratory for Physical Sciences — Amorphous dielectrics are prevalent in lithographic circuits, but their presence can decouple superconducting qubits. We investigate the relationship between stoichiometry and low-temperature loss in silicon nitride dielectric films, where two-level system defects are unsaturated. The silicon nitride films are deposited by plasma-enhanced chemical vapor deposition at 300 degrees celsius, with silane and nitrogen as precursor gases. The precursor gas ratio is changed and film density, crystalline order, stress, and hydrogen incorporation are measured. Hydrogen, purity of the substrates and metals used in the process but also to the details of the fabrication. We measure 1/f noise spectra in dc SQUID phase qubits using a microwave reflectometry technique. One of the SQUID junctions is shunted by a large capacitor, forming a microwave frequency resonator biased and driven to show nonlinear response, typically at 1.5 GHz. This nonlinearity means small current or flux fluctuations produce large changes in reflected phase which we can measure using homodyne detection. Measurements from aluminum qubits on sapphire are compared to previous measurements of 1/f noise flux in SQUIDs and a similarly designed Nb/AIOx/Nb on silicon dc SQUID fabricated by Hynes; data was taken at temperatures ranging from 50 mK to 500 mK.

This research was supported by JQI, CNAM and LPS.

4:06PM T17.00007 Low-photon number studies of inductively-coupled superconducting resonators, MOE KHALIL, Laboratory for Physical Sciences and University of Maryland, Department of Physics, HANHEE PAIK, Laboratory for Physical Sciences, FRED WELLSTOOD, University of Maryland, Department of Physics, KEVIN OSBORN, Laboratory for Physical Sciences — Quality factors near one million have been observed in on-chip superconducting resonators for many years, but new studies on resonators reveal much lower quality factors at low-photon numbers, perhaps due to the presence of anomalous two-level system defects. We have designed and fabricated four new aluminum thin-film resonator types near 6 GHz. They include a lumped-element resonator, a slot-line resonator, and two hybrids, both of which contain a slot line and either an inductor or a capacitor. The resonator types have a consistent line width and are fabricated on a sapphire substrate to facilitate the study of surface defects, such as two-level systems. We plan to compare their quality factors in an effort to better understand the loss mechanism associated with the surface. All the resonator types have inductive coupling to a coplanar waveguide with geometrical symmetry that can be used to construct useful Josephson junction resonators.

This research was supported by the National Security Agency.
4:18PM T17.00008 LC Filtered dc SQUID Phase Qubit with Low Dielectric Loss\textsuperscript{1}, HYEOKSHIN KWON, A. J. PRZYBYLSZ, University of Maryland, College Park — We have investigated a dc SQUID phase qubit with LC filter, which has a relatively small (\sim 4 \mu m^3) Al/AIO\textsubscript{x}/Al Josephson junction shunted by an additional capacitor built using low-stress thin film SiN\textsubscript{x}. The LC isolation provides an additional isolation factor at the junction plasma frequency and allows flexibility in the choice of SQUID parameters. We report Rabi oscillations with a 42 ns envelope decay time (T\textsubscript{1}), and a 32 ns energy relaxation time (T\textsubscript{1}), consistent with a loss tangent of about 7 \times 10^{-4} in the loss-stress SiN\textsubscript{x}. We also report on progress towards getting longer coherence times using a high-stress SiN\textsubscript{x} with a lower loss tangent.

\textsuperscript{1}Funding provided by JQI, CNAM and the DOD.

4:30PM T17.00009 Microwave response of vortices in Al and Re superconducting thin films\textsuperscript{1}, C. SONG, T.W. HEITMANN, M.P. DEFEO, K. YU, B.L.T. PLOURDE, Syracuse University, R. MCDERMOTT, University of Wisconsin, M. NEELEY, J.M. MARTINIS, UC Santa Barbara — Vortices trapped in superconducting microwave resonant circuits contribute excess loss and can result in substantial reductions in the quality factor. Thus, characterizing the microwave vortex response in superconducting thin films is important for the design of superconducting qubits, which are typically operated in small, but non-zero, magnetic fields. By cooling in fields of the order of 1 Gauss and below, we have characterized the magnetic field and frequency dependence of the microwave response of a small density of vortices in resonators fabricated from thin films of Re and Al. Above a certain threshold cooling field, vortices become trapped in the resonators and vortices in the Al resonators contribute greater loss and are influenced more strongly by flux creep effects than in the Re resonators. This different behavior can be described in the framework of a general vortex dynamics model related to the interplay between the vortex pinning in the films and the flux-flow viscosity.

\textsuperscript{1}Supported by NSF DMR-0547147

4:42PM T17.00010 One- and two-photon spectroscopy of a flux qubit coupled to a microscopic defect, ADRIAN LUPASCU\textsuperscript{2}, PATRICE BERTET\textsuperscript{2}, EDUARD DRIESSEN\textsuperscript{3}, KEES HARMANS, HANS MOOIJ, Delft University of Technology, The Netherlands, QUANTUM TRANSPORT GROUP TEAM — We observed the dynamics of a superconducting flux qubit coupled to a microscopic defect. The presence of the defect is visible as an anticrossing in the spectroscopy of the flux qubit, as measured using one-photon excitation. We analyze the energy-level structure of the combined qubit-defect system using both one- and two-photon spectroscopy. The use of two-photon spectroscopy allows us to extract important additional information about the anharmonicity and coupling of the defect. We find that the system coupled to the qubit can be a two-level system, but not a harmonic oscillator. We consider two basic models, for a microscopic defect which is coupled to the qubit either magnetically or electrically respectively. We conclude that the large coupling constant, of approximately 200 MHz, can only be accounted for by electric coupling, and not by magnetic coupling. This shows that electrically coupled microscopic two-level systems are relevant to decoherence of superconducting flux qubits.

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\textsuperscript{2}Present address: CEA Saclay, France
\textsuperscript{3}Present address: University of Leiden, The Netherlands

4:54PM T17.00011 Probing anomalous two-level systems with a Cooper-pair box\textsuperscript{1}, BENJAMIN PALMER, Laboratory for Physical Sciences — We have used a Al/AIO\textsubscript{x}/Al Cooper-pair box (CPB) qubit to detect coupling to anomalous “two-level” quantum systems. By measuring the excitation spectrum and lifetime of the first excited state from 15 GHz to 50 GHz of the CPB at a temperature of 40 mK, one can identify anomalous levels and ascertain the magnitude of the quantum noise that is coupled to the qubit. It was found that the frequency of a distinct avoided level crossing depends on gate voltage and the size of the splitting depends on the effective Josephson energy. Both the gate voltage and Josephson energy dependence are consistent with coupling to extraneous charged two-level systems formed by point charges that can tunnel between two positions in the oxide of the Josephson junction. By fitting a model Hamiltonian to our data, we are able to extract microscopic information about the charge fluctuator such as the well asymmetry (\sim 130 micro-eV), tunneling rate (\sim 8 GHz) and a minimum hopping distance for the charge fluctuators (\sim 0.8 Angstroms).

\textsuperscript{1}This research was supported by the National Security Agency.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T18 DPOLY: Focus Session: Organic Photovoltaics and Other Photonic Devices

2:30PM T18.00001 Surface plasmon polariton assisted organic solar cells, P. PEUMANS, Stanford U. — No abstract available.

3:06PM T18.00002 Harvesting Lost Photons: Minimizing Sub-Bandgap Losses in Organic Photovoltaic Devices by Up-conversion, CLARA SANTATO, LORANGER SEBASTIAN, BANVILLE DAVID, Genie Physique/Polytechnique Montreal, ROSEI FEDERICO, EMT-IRIS/Varennes, PEREPICHKA DMIYTRO, McGill/Chemistry — We report on a novel approach to increase the efficiency of organic photovoltaic (OPV) cells in the near-infrared region of the solar spectrum by blending the organic semiconductors with rare-earth doped nanoparticles. The approach consists in (i) synthesizing lanthanide-doped nanoparticles capable of efficient energy transfer of organic photovoltaic (OPV) cells in the near-infrared region of the solar spectrum by blending the organic semiconductors with rare-earth doped nanoparticles and (ii) assembling these nanoparticles, in blends with p-type polythiophenes and n-type fullerences, in solution-processed OPV cells capable to harvest NIR photons.

3:18PM T18.00003 In-situ X-ray characterization of thermal and solvent based annealing of thin P3HT and P3HT/PCBM films\textsuperscript{1}, TOMMY HOFMANN, Brookhaven National Laboratory, HTAY HLAING, Stony Brook University, CHANG-YONG NAM, CHARLES BLACK, BENJAMIN OCKO, Brookhaven National Laboratory, BROOKHAVEN NATIONAL LAB TEAM — We have studied the annealing of thin films of P3HT (poly(hexyloxyphopene) and mixed P3HT and PCBM thin films using in-situ Grazing Incidence Angle x-ray scattering techniques at the National Synchrotron Light Source. The films, 50-200 nm thick, were prepared using spin coating from a volatile solution. Both thermal and solvent annealing techniques are well known to improve electrical properties yet the precise mechanism is not well understood. In our measurements, we have monitored the dependence of the diffraction peak positions and widths under a variety of different in-situ thermal and solvent conditions. A detailed comparisons between these methods provides new insight into how to improve the crystallinity beyond what can be obtained by thermal methods alone. This may eventually lead to better electrical properties in thin film organic photovoltaic devices.

\textsuperscript{1}This work is supported by the U.S. DOE Contract No. DE-AC02-98CH10886 and a Brookhaven National Laboratory LDRD Project.
3:30PM T18.00004 Excited-State Dynamics at Organic Photovoltaic Heterojunctions by Pump-Probe Photoelectron Spectroscopy. GREGORY DUTTON, DANIEL DOUGHERTY, National Institute of Standards and Technology, WEI JIN, WILLIAM CULLEN, JANICE REUTT-ROBEY, University of Maryland, STEVEN ROBEY, National Institute of Standards and Technology — The critical process of charge separation in organic photovoltaic (OPV) devices is determined directly at the organic heterojunction, but these interfaces have been less extensively studied than organic/metal interfaces. We prepare model photovoltaic heterojunctions by deposition of ultrathin films of organic semiconductors on single-crystal metal substrates. The electronic structure of the component materials and their interfaces is determined with ultraviolet photoelectron spectroscopy (UPS) and two-photon photoemission (2PPE). The systems studied in this work involve phthalocyanines and analogs as donors and C60 fullerene as acceptor. Time-resolved pump-probe experiments are applied to directly measure the excited state dynamics at these OPV heterojunctions. An ultrafast visible pump pulse selectively generates excitons in one material, followed by a time-delayed UV probe to interrogate the population of the acceptor charge transport level. Analysis of cross-correlations reveals the timescales of charge separation and recombination at the interface. Additionally, comparison will be made to structural and local spectroscopic studies of similar phthalocyanine/fullerene systems made by STM/STS.

3:42PM T18.00005 The role of triplet excitons in enhancing polymer solar cell efficiency: a photo-induced absorption study. KAI YANG, SUCHI GUHA, Department of Physics and Astronomy, University of Missouri-Columbia, MO 65211 — Inclusion of heavy metal atoms in a polymer backbone allows transitions between the singlet and triplet manifolds. Interfacial dissociation of triplet excitons constitutes a viable mechanism for enhancing photovoltaic (PV) efficiencies in polymer heterojunction-based solar cells, which are now becoming feasible options for solar panels. The PV efficiency from polymer solar cells utilizing a ladder-type poly para phenylene polymer (PhLPPP) with trace quantity of Pd atoms and a fullerene derivative (PCBM) is almost 10 times more than its counterpart (MeLPPP) with no Pd atom. Evidence is presented for the formation of a weak ground-state charge-transfer complex (CTC) in the blended films of PhLPPP and PCBM, using photo-induced absorption (PIA) spectroscopy. Such complexes are not seen in the PIA spectrum of MeLPPP. PCBM blends. Possible mechanisms for the CTC state formation as well as the significance of this to the understanding and optimization of polymer blended solar cells will be discussed.

3:54PM T18.00006 Photophysics of charge-transfer excitons in thin films of π-conjugated polymers. DEMETRA PSIACHOS, SUMIT MAZUMDAR, University of Arizona — We develop a theory of the electronic structure and photophysics of interacting chains of π-conjugated polymers to understand the differences between solutions and films. While photoexcitation generates only the intrachain exciton in solutions, the optical exciton as well as weakly allowed charge-transfer excitons are generated in films. We show that a significant fraction of ultraviolet photoinduced absorptions (PAs) in films originate from the lowest charge-transfer exciton. Using sophisticated many-body approaches that take into account high order configuration interaction, we have calculated the full wavelength-dependent PA spectra of pairs of interacting PPV oligomers. Good qualitative agreement is obtained with the experimental PA spectra of thin films of π-conjugated polymers. The origin of each individual PA is explained within our theory. Our work resolves long-standing controversies regarding the nature of the primary photoexcitations in films.

4:06PM T18.00007 Photo-crosslinkable Polythiophenes for Efficient Thermally Stable Organic Photovoltaics. BUMJOON KIM, KAIST and UC Berkeley, YOSHI MIYAMOTO, BIWU MA, JEAN M.J. FRECHET, UC Berkeley — We report a new series of bromine-functionalized poly(3-hexylthiophene) (P3HT-Br) copolymers for use in solution processed organic photovoltaics (OPVs). P3HT-Br copolymers were synthesized from two different monomers, where the ratio of the monomers was carefully controlled to achieve a UV photo-crosslinkable layer while leaving the π−π stacking feature of conjugated polymers unchanged. Photo-crosslinkable P3HT-Br was demonstrated as effective electron donors in OPVs. The crosslinking stabilizes P3HT-Br/PCBM blend morphology preventing the macro phase separation between two components, which lead to OPVs with remarkably enhanced thermal stability. The drastic improvement in thermal stabilities is further characterized by microscopy as well as grazing incidence X-ray scattering (GIXS). The use of these copolymers for solution processed efficient bilayer PVs is also described. Benefited from the little disturbance in π−π stacking by crosslinkable units as evidenced in GIXS, P3HT-Br/PCBM bilayer device shows high power conversion efficiency at over 2.2% and excellent thermal stability.

4:18PM T18.00008 Temperature Dependence of Biexciton Decay and Intermolecular Hopping in Zinc Phthalocyanine Films. CHRISTOPHER RYAN, Graduate Student — The femtosecond exciton dynamics of melt-pressed zinc phthalocyanine (ZnPc) films are studied in the temperature range of 90-400 K. In this range ZnPc goes through a transition from a crystalline solid to a liquid crystalline phase. For the entire temperature range, the excitons are shown to decay on the time scale of 10's of picoseconds, and these dynamics are nonlinear with respect to pump fluence. Such a behavior is well described by a biexciton recombination model under one dimensional diffusion constraints. The single exciton lifetime and the biexciton recombination crosssection are extracted at all temperatures. From the latter, the exciton hopping time is calculated. The exciton hopping time decreases with temperature in the crystalline phase, but increases in the liquid crystalline phase. The role of temperature and structural exciton hopping time will be discussed.

4:30PM T18.00009 White tandem OLED with carbon nanotube interlayer. ALEXIOS PAPADIMITRATOS, SolarInc, Nanotech UT Dallas, RAQUEL OVALLE ROBLES, RAY BAUGHMAN, Nanotech UT Dallas, ANVAR ZAKHIDOV, Solar Inc, Nanotech UT Dallas — White organic light emitting diodes (OLEDs) have become well recognized as an important candidate for future lighting and display applications. An exciting idea to generate white color places R, G, B pixels in a side-by-side geometry. Also, white tandem OLEDs have been developed by vertically stacking in series multiple electroluminescent layers. However, such structures require a complex interfacial layer which is usually fabricated by strong dopants to form a p+/n− interface. We have shown earlier that transparent carbon nanotubes (CNT) can be used as effective three dimensional charge injectors in polymer light emitting diodes[1] and OLEDs[2]. Now, we show that CNT can be used as an interlayer in two cell OLEDs with complimentary colors. We show that tandem devices with CNT interlayers, together with selective barriers and PEDOT:PSS coating can control the device color. In addition, the emission intensity can be controlled by independently tuning the driving voltage and current. In the case of overdoped p+/n− interlayers we do not have this opportunity which is a great advantage of CNT injectors. We also compare the performance of multilaw CNTs vs. that of single wall CNTs in the tandem OLEDS. [1]R-H.Baughman et al.Scienc, 297,787-792(2002).[2]C.D.Williams et al.Appl. Phys. Lett. 93,183506(2008).

This work was supported by NSF-ECSS0824563

This work was supported by NSF-DMR-0705163.
4:42PM T18.00010 Tuning optical properties of blue-emitting polyfluorenes via hydrostatic pressure, KESHAB PAUDEL, MEERA CHANDRASEKHAR, SUCHI GUHA, Department of Physics and Astronomy, University of Missouri- Columbia, MO 65211 — Polyfluorenes (PFs) represent a unique class of poly para-phenylene based blue-emitting polymers with intriguing structure-property relationships. Slight variations in the choice of functionalizing side chains result in dramatic differences in the inter- and intra-chain structures in PFs. Highlighting these differences are two prototypical PFs, poly (9,9-di (n, n-octyl) fluorene) (PF8) and poly (9,9-di ethyl- hexyl) fluorene) (PF2/6). In addition to the nematic liquid crystal (n- LC) mesophase, PF8 is characterized by at least five structural phases. We present photoluminescence (PL) and Raman scattering studies of powder samples and thin films of PF8 under hydrostatic pressure. The powder sample was thermally annealed at 2GPa. The PL vibronics of the as-is powder sample red-shift at an average rate of 30 meV/GPa whereas the thermally annealed sample red-shifts at a higher rate of 50 meV/GPa, indicating a different crystalline mesophase for the annealed sample. The Huang-Rhys factor is found to increase with increasing pressures signaling a higher geometric relaxation of the electronic states. The Raman peaks harden with increasing pressures; the intra-ring C-C stretch frequency at 1600 cm$^{-1}$ has a pressure coefficient of 5 cm$^{-1}$/GPa and exhibits asymmetric line shapes at higher pressures.

4:54PM T18.00011 SERS Characterization of Self-Assembled Monolayers Embedded on Plasmonic Nano-structure, MASATO MAITANI, Materials Science and Engineering, Penn State University (Penn State), DOUGLAS OHLBERG, Information & Quantum Systems Laboratory, Hewlett-Packard Laboratories, Palo Alto, CA (Hewlett-Packard), HAEYOUNG YOON, Electrical Engineering (Ee), Penn State, PING KAO, Ee, Penn State, DEMIREL MELIK, Engineering Science and Mechanics, Penn State, ZHIYONG LI, DUNCAN STEWART, STANLEY WILLIAMS, Hewlett-Packard, THERESA MAYER, Ee, Penn State, DAVID ALLARA, Chemistry, Penn State — We discuss Raman spectroscopic analysis of self-assembled monolayers embedded in two different types of nano-structures capable of sustaining localized surface plasmon-surface plasmon polariton coupling via nanoscale gaps and curved surface features. Both structures consist of metal-molecule-metal (M-M) junctions which can also allow charge transport through the molecular gaps. Our results indicate different electromagnetic and charge transport characteristics as a function of the top metal-molecule chemical interaction. We also report direct correlations between charge transport states, SERS response and inelastic vibrational scattering in selected M-M electronic device junctions.

5:06PM T18.00012 Non-linear optical and local-field factors in liquid chloroform: A time-dependent density-functional theory study, DAVID A. STRUBBE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory, XAVIER ANDRADE, ANGEL RUBIO, European Theoretical Spectroscopy Facility, Universidad del Pais Vasco and Centro Mixto CSIC-UPV/EHU, San Sebastian, Spain, STEVE G. LOUIE, Department of Physics, University of California, Berkeley, and Materials Sciences Division, Lawrence Berkeley National Laboratory — Chloroform is often used as a solvent and reference when measuring non-linear optical properties of organic molecules. We calculate directly the non-linear susceptibilities of liquid chloroform at optical frequencies, using molecular dynamics and the Sternheimer equation in time-dependent density-functional theory [X. Andrade et al., J. Chem. Phys. 126, 184106 (2007)]. We compare the results to those of chloroform in the gas and solid phases, and experimental values, and make an ab initio calculation of the local-field factors which need to extract molecular properties from liquid calculations and experimental measurements.

5:18PM T18.00013 Time resolved photoluminescence studies of long lived emissive specie in F8BT:PFB blends, SIMON GÉLINAS, Regroupement Quebecois sur les Materiaux de Pointe, Departement de Physique de l’Universite de Montreal, IAN HOWARD, RICHARD FRIEND, Cavendish Laboratory, University of Cambridge, CARLOS SILVA, Regroupement Quebecois sur les Materiaux de Pointe, Departement de Physique de l’Universite de Montreal — Type-II heterojunctions play a crucial role in organic optoelectronic devices. We use donor-acceptor polyfluorene blends as a model system to understand excited-state dynamics at heterojunctions. These interfacial excitations are intrachain singlet and triplet excitons, geminate polaron pairs, and exciplexes (interfacial charge-transfer excitons). Time-resolved photoluminescence (PL) spectra were taken at 10 K and room temperature to investigate the interconversion dynamics of these species. We observe delayed PL with sub-linear excitation fluence dependence. This implies that delayed singlet exciton generation involves a bimolecular annihilation mechanism. By means of kinetic modeling, we propose triplet-triplet exciton annihilation as a regeneration route to singlet excitons, and subsequently to exciplexes. This points to a significant (< 15 %) yield of triplet excitons after interfacial charge separation, and to the central role of these species on the interfacial dynamics.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T19 DPOLY: Theory and Simulation II 320

2:30PM T19.00001 Theory of polyzwitterionic solutions, RAJEEV KUMAR, GLENN FREDRICKSON, Materials Research Lab, UCSB — Conformations of polyzwitterionic molecules in aqueous solutions are investigated using the variational method. We have carried out self-consistent calculations for the degree of counterion adsorption on the zwitterionic sites and the size of a single polyzwitterionic chain. These calculations are used to analyze the solubility of these molecules in water. Results for the effect of an asymmetric counterion adsorption, electrostatic interaction strength, salt concentration, solvent quality, specificity of the zwitterionic monomeric units and the added salt on the conformations of the polyzwitterionic chain will be presented.

2:42PM T19.00002 Charge transport in conjugated polymers: a multiscale picture, VICTOR RUEHLE, Max Planck Institute for Polymer Research, JAMES KIRKPATRICK, Imperial College London, KURT KREMER, DENIS ANDRIENKO, Max Planck Institute for Polymer Research — A framework to study charge transport in conjugated polymers using realistic morphologies is developed. First, the atomistic force field is refined using first-principles calculations. Systematic coarse graining is then performed to extend simulation times and system sizes accessible to molecular dynamics simulations. Material morphologies are generated using the coarse grained and atomistic models. Finally, the charge mobility is obtained using temperature activated hopping picture for charge transport [1]. The framework is tested on neutral and oxidized polyppyrole with different structural ordering [2].


DPG is acknowledged for the financial support
2:54PM T19.00003 First principles electronic properties investigation of polythienoacene and its derivatives1. SIMON PESANT, PAUL BOULANCER, GUILLAUME DUMONT, MICHEL CÔTÉ, Département de physique et Regroupement québécois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — The electronic properties of ladder-type polythiophene (polythienoacene) and its derivatives are studied using density functional theory. Upon an analysis of the variation of the band gap when comparing the non-ladder and the ladder-type polymers, a discrepancy is found between the thiophene and the pyrrole(nitrogen-substituted thiophene) polymer families. The polythienoacene has a larger band gap than the polythiophene whereas the opposite is found for the pyrrole polymers. Also, it is found that a simple alternation of the sulfur atom in polythienoacene structure by nitrogen or boron atoms can lead to small band gap polymers. The excitations of these polythienoacene’s derivatives are investigated using time-dependent density functional theory.

1This work was supported by grants from the FQRNT and CRSNG. The computational resources were provided by the Réseau québécois de calcul de haute performance (RQCHP).

3:06PM T19.00004 Electronic structure and carrier transport in disordered conjugated polymers1. NENAD VUKMIROVIC, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Thin films of realistic conjugated polymer materials contain both crystalline and amorphous regions, where the latter ones are less understood. This study was therefore focused on electronic structure and carrier transport in amorphous regions of polythiophene (PT) and poly(3-hexylthiophene) (P3HT). Atomic structures were obtained from classical molecular dynamics using a simulating annealing procedure and the charge patching method [1] was used to calculate the electronic structure. It was found that disorder in the electronic structure of P3HT comes from disorder in the conformation of individual chains, while in case of PT there is an additional contribution due to disorder in electronic coupling among the chains [2]. The electron-phonon coupling matrix elements in P3HT were also calculated and carrier mobility due to phonon-assisted hopping was estimated.

1This work was supported by the DMS/BES/SC of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. It used the resources of National Energy Research Scientific Computing Center (NERSC).

3:18PM T19.00005 Ab initio Study of Diketo-Pyrrolo-Pyrole Polymers for Photovoltaic Applications1. SIMON LÈVESQUE, JEAN FRÉDÉRIC LAPRADE, MICHEL CÔTÉ, Département de physique et Regroupement québecois sur les matériaux de pointe (RQMP), Université de Montréal, Canada — Using density functional theory with the hybrid functional B3LYP, we investigate the electrical and optical properties of polymers made with diketo-pyrrolo-pyrole. It is found that the value of the band gap can be tuned by varying the number of thiophene units within the polymer. Band structure and time-dependent density functional theory results will also be presented.

1We are grateful to Mario Leclerc for helpful discussion. This work is supported by NSERC. Computational resources were provided by the RQCHP.

3:30PM T19.00006 First-principles investigation of PVDF and its copolymers, V. RANJAN, LI-PING YU, North Carolina State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, North Carolina State University, Raleigh, NC and Oak Ridge National Laboratory, TN — Recently, PVDF and its copolymers have generated significant interest due to their electroactive properties [1] and potential for ultra-high energy-storage applications [2]. In this talk, we present the results of first-principles calculations of stable phases and dielectric properties of different copolymers and terpolymers of PVDF at varying concentrations. Our results show that at very high concentrations of Chloro-trifluoroethylene (CTFE), PVDF/CTFE displays sharp transitions between non-polar (α) and polar (β) phases. On the contrary, the same transitions in copolymers with trifluoroethylene (TrFE) and tetrafluoroethylene (TeFE) are not sharp and happen at lower concentrations. We discuss the interplay of copolymer admixture on the dielectric properties of PVDF and discuss the suitability of copolymers for energy storage and electroactive applications. [1] S. G. Lu et al., App. Phys. Lett. 93, 042905 (2008). [2] V. Ranjan et al., Phys. Rev. Lett. 99, 047801 (2007).

3:42PM T19.00007 Adaptive Tempering Monte Carlo Study of Dense Polypyrrole Systems1. YAFEI DAI, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 20030 — A modified rigid-ion polarizable model potential of polypyrrole is developed with parameters fitted on multiple points of the electronic energy surface of pyrrole oligomers (n-Py) of different sizes calculated with a hybrid density functional approach [1]. Using this potential, systems containing 192 chains (4-Py) and 64 chains (12-Py) were structurally optimized with the Adaptive Tempering Monte Carlo algorithm [2]. Energetics and structure of these systems were studied as a function of density. Both systems have characteristics of a liquid for densities in the range 0.66–1.09 g/cm³, and a critical value. We propose a scaling relation for this case, in agreement with self consistent field theory for (σf = σg). 1Computational support from Teragrid grant PHY0500026.

3:54PM T19.00008 Effect of the chain length and segment size of the free polymer on the interaction between two grafted monolayers in a good solvent, WALTER CHAPMAN, SHEKHAR JAIN, Rice University, VALERIY GINZBURG, PRASANNA JOG, JEFFREY WEINHOLD, RAKESH SRIVASTAVA, Dow Chemical Company, ISAF DFT COLLABORATION — The interaction between two polymer grafted surfaces is important in many applications, like nanocomposites, colloid-stabilization, and polymer alloys. In our previous work [Jain et. al., J. Chem. Phys. 126, 154910 (2008)], we showed that interfacial statistical associating fluid theory (iSAFT) density functional theory (DFT) successfully calculates the structure of the grafted polymer chains in the absence/presence of free polyatomic solvent. In the current work, we have applied iSAFT to calculate the force of interaction between two such grafted monolayers in implicit good solvent conditions. In particular, we have considered the case where the segment sizes of the free (σf) and grafted (σg) polymers are different. The interactions between the two monolayers in the absence of the free polymer is always repulsive. However, in the presence of free polymer, the force can be either purely repulsive or can have an attractive minimum depending upon the relative chain lengths of the free (Nf) and grafted polymers (Ng). The attractive minimum is observed only when the ratio, Nf/Ng, is greater than a critical value. We propose a scaling relation for this case, in agreement with self consistent field theory for (σf = σg).
can be extended to study longer n-alkane molecules and the change of nucleus conformation as n increases. This method is able to calculate the end and side surface free energies of a cylinder nucleus model from the simulation data without making further assumption. This method was developed using simulation techniques. The adiabatic nucleation trajectory was then sampled using the Monte Carlo umbrella sampling technique. The surface energy of the crystal nuclei depends on the properties of the final product. In this work we report the results of molecular simulations of crystal nucleation of n-alkanes from the melt. A realistic model of the final product is used where the connectivity could produce very different crystal nucleus conformations, which are important factors in determining the subsequent crystal growth process and the properties of the final product. These models to characterize the Helmholtz energy of the repulsive reference fluids (A0) along with the first and second order perturbation contributions (A1, A2) as functions of density and composition. Taken together, these terms generate a complete equation of state for the mixture, including temperature effects as well as density and composition. The specific hydrocarbons studied were methane, ethane, propane, n-butane, n-hexane, n-heptane, n-decane, and benzene. The specific alcohols were water, methanol, ethanol, n-propanol, and n-octanol. Unfortunately, a slight inconsistency was encountered when the trend observed for these small molecules was extrapolated to the long chain limit. Therefore, we extend the analysis to mixtures of n-alkanes, branched hydrocarbons, and aromatics with polymeric molecules of: n-alkanes, ethyl-styrenes, ethyl-proplyenes, and isoprenes. The perturbation contributions can be accurately characterized by van der Waals mixing rules and compared with the MCSL SAFT and Guggenheim-Staverman theories.

The authors gratefully appreciate ChemStations, Houston, TX for financial funding.

5:18PM T19.00010 ABSTRACT WITHDRAWN —

4:30PM T19.00011 Simulation of Microheterogeneous Networks and Extraction of Segment Orientation Behavior from D-NMR Spectra — BERNARDO AGUILERA-MERCADO, CLAUDE COHEN, FERNANDO ESCOBEDO, School of Chemical and Biomedical Engineering, Cornell University — The degree of heterogeneity in the microstructure of end-linked elastomer networks has been shown to have a very strong impact on the network mechanical and elastic properties such as: ultimate strain, modulus, and toughness. Networks with crosslinks and chains inhomogeneously distributed are expected to exhibit heterogeneous segment orientation responses. The global segment orientation of systems with frozen inhomogeneities, and a significant amount of highly stretched chains at the unperturbed state, cannot be captured by measurements of the deuterium NMR spectra alone. Spectrum frequency splits quantify the segment orientation in terms of partial excluded volume interactions only and do not account for the contributions arising from large end-to-end chain deformations. Long wings of the spectrum reflect the presence of strongly aligned segments ignored when one considers only the split. A new methodology based on the Maximum-Entropy method is proposed to find the probability density of an order parameter that describes the network segment orientation from which the global orientation behavior can be completely characterized. The methodology is validated with both molecular simulation and experimental data.

4:42PM T19.00012 Cooperative dynamics in polymer melts: a comparison of theoretical predictions with Neutron Spin Echo experiments — MARINA GUENZA, University of Oregon — We present a comparison between theoretical predictions of the Generalized Langevin Equation for Cooperative Dynamics (CDGLE) and Neutron Spin Echo data of dynamic structure factors for polystyrene melts. Experiments, performed by Zamponi and coworkers, cover an extended range of length- and time-scales providing a compelling test for the theoretical approach. Samples investigated include chains with increasing molecular weights, undergoing dynamics across the unentangled to entangled transition. Measured center-of-mass mass-square displacements display a crossover from subdiffusive to diffusive dynamics. The Generalized Langevin Equation for Cooperative Dynamics relates this anomalous diffusion to the presence of the interpolymer potential, which correlates the dynamics of a group of slowly diffusing molecules in a dynamically heterogeneous liquid. Theoretical predictions of the subdiffusive behavior, its crossover to free diffusion, and of the number of macromolecules undergoing cooperative motion are in qualitative agreement with experiments.

4:54PM T19.00013 Equilibrium Partitioning of Polymers between Bulk Dilute Solution and Confining Pores — YANWEI WANG, FLEMMING Y. HANSEN, GUENTHER H. PETERS, OLE HASSAGER, Technical University of Denmark — We have developed a novel framework [1] for the description of the steric hindrance effect on polymers that are subject to confining geometries. The two main ingredients are (i) a new computational method, the Confinement Analysis from Bulk Structures (CABS) approach, which enables calculation of the equilibrium partition coefficient (pore-to-bulk concentration ratio) as a function of the confinement size solely based on snapshots of polymer configurations in bulk, and (ii) the definition of a new molecular size parameter, the steric exclusion radius, which permits collapsing all partition coefficient data for different polymers in the weak confinement regime onto a universal curve. Our latest development in extending the CABS method to cylindrical and spherical pores will be presented.

5:06PM T19.00014 Multivalent Nanoparticles: adsorption and organization of bidisperse polymer chains onto a solid interface — FOLUSHO OYEROKUN, RICHARD VAIA, JOHN MAGUIRE, BARRY FARMER, AFRL — Multivalent nanoparticles, i.e. nanoparticles with two or more ligands attached to their surfaces, are used in a variety of scientific and technological applications. The most common protocols for synthesizing these multivalent nanoparticles involves immersion of the particles into a solution containing the various ligands or into a solution containing an excess of one ligand to drive a partial (solvent mediated) exchange reaction with a previously bound ligand. Despite intense experimental activities, the dependence of the surface coverage on free ligand concentration and solvent quality is still poorly understood. This study addresses the thermodynamics of adsorption of bidisperse end-functionalized polymer chains in a good solvent onto a flat surface. At equilibrium, the absorbed chains form a bidisperse polymer brush in contact with the solution. The role of the degree of bidispersity, adsorption energy, solvent quality on monomer concentration profile, brush height and degree of penetration of free short and long chains into the brush layer will be discussed.

5:18PM T19.00015 Molecular simulation of crystal nucleation of n-alkane melts — PENG YI, GREGORY RUTLEDGE, Massachusetts Institute of Technology — The homogeneous nucleation of a crystal phase is one of the most interesting phenomena of molecular fluids, yet the microscopic mechanism of which still remains poorly understood. It is even more a mystery in chain molecule systems because the chain connectivity could produce very different crystal nucleus conformations, which are important factors in determining the subsequent crystal growth process and the properties of the final product. Our latest development in extending the CABS method to cylindrical and spherical pores will be presented. The adiabatic nucleation trajectory was then sampled using the Monte Carlo umbrella sampling technique. The surface energy of the crystal nuclei was calculated assuming a spherical nucleus model and compared with previous studies to validate our numerical definition of a crystal nucleus. We were also able to calculate the end and side surface free energies of a cylinder nucleus model from the simulation data without making further assumption. This method can be extended to study longer n-alkane molecules and the change of nucleus conformation as n increases.
2:30PM T20.00001 Magnetoresistance and magnetic-field-effects in organic semiconductor devices.

MARKUS WOHLGENANNT, U. of Iowa — No abstract available.

3:06PM T20.00002 Photo-induced Magnetism and Spintronics in Organic Semiconductors

JUNG WOO YOO, The Ohio State University — Recent years have witnessed growing attention on manipulating spins in organic species. One of the interesting phenomena in organic-based magnets is controlling magnetic properties by optical stimulus, a property not exhibited in metallic magnets. Three classes of known phenomena and mechanism will be discussed: i) manipulation of number of spins by optically induced charge transfer in cyanide-bimetallic complexes [1], ii) phenomenon in organic-based magnets is controlling magnetic properties by optical stimulus, a property not exhibited in metallic magnets. Three classes of

JUNG WOO YOO

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In collaboration with A. J. Epstein and V. N. Prigodin (The Ohio State University)

3:42PM T20.00003 Magnetic properties of TCNQF4 reacted with Ni(cod)2 reacted with Ni(cod)2, IAN TERRY, KIMBERLY QUINN, MAREK SZABLEWSKI, Department of Physics, Durham University, Durham, DH1 3LE, UK — Recently it was reported that a room temperature ferromagnetic material (TC=400K), Ni2TCNQ, was synthesized by reacting the organic acceptor tetracyanoquinodimethane (TCNO) with bis(1,5 cyclooctadiene) nickel (Ni(cod)2)[1]. In the present work we report the magnetic properties of a material which was synthesized following the same chemical route as that of Ni2TCNQ, except tetrafluoro-tetracyanoquinodimethane (TCNOF4) was used instead of TCNQ. The new metal-organic compound shows qualitatively similar magnetic properties to Ni2TCNQ, with ferromagnetic behavior being observed at room temperature. The specific magnetic properties can be described by assuming that there is both a paramagnetic and ferromagnetic phase in the material, with the ferromagnetic phase having a measured Curie temperature of about 620K, close to that of nickel. TEM and XRD data provide evidence for the existence of nickel nanoparticles within the material. We conclude that nickel nanoparticles are produced during the synthesis and are probably responsible for ferromagnetic properties observed at room temperature. 1.R. Jain et al, Nature 445, 291, (2007).

3:54PM T20.00004 Magnetic and surface studies of transition metal complexes for molecular spintronics

PATRICK TRUITT, RAMAN TALWAR, EZEKIEL JOHNSTON-HALPERIN, Dept. of Physics, The Ohio State University, NORBANI ABDULLAH, Dept. of Chemistry, University of Malaya, CARLY REED, NAMRATA SINGH, CHANDRANI CHATTERJEE, MALCOLM CHISHOLM, Dept. of Chemistry, The Ohio State University — We have synthesized organometallic complexes consisting of a transition metal ion chelated by amphiphilic ligands. This talk will focus on efforts to assess the suitability of these molecules for the creation of magnetically active monolayers via the Langmuir-Blodgett technique. The paramagnetic nature of the molecules is probed by SQUID magnetometry and EPR spectroscopy, demonstrating that the spin magnitude can be varied by chemical substitution of the transition metal ion. To study monolayer formation ability, the molecules are spread on a Langmuir trough and pressure-area isotherms are recorded under compression. Attempts to deposit monolayers onto substrates and to make electrical contact for transport measurements will also be discussed.

4:06PM T20.00005 Magneto-Transport in Polyaniiline Nanofiber Network

K. DENIZ DUMAN, N.-R CHIOU, V.N. PRIGODIN, Dept. of Physics, The Ohio State University, Columbus, Ohio, A. J. EPSTEIN, Dept. of Physics, Dept. of Chemistry, The Ohio State University, Columbus, Ohio — We report large magnetoresistance (up to 2% at 8 T and 3 K) for polyaniline nanofiber network composed of nanofibers with an average diameter of about 80 nm. The polyaniline nanofiber networks were synthesized via chemical oxidative polymerization [1] and were studied at low and high electric and magnetic fields for temperatures 2 K- 250 K for their magneto-transport behavior. A transition from positive MR (temperatures 75 K and below) to negative MR (temperatures 100K and above) is observed. The MR may be explained by possible competing mechanisms; shrinkage of the hopping wavefunction and quantum interference effect in the applied magnetic field. It is also noted that applied electric field affects MR. In the positive MR regime an increase in MR is observed as the applied electric field decreases. Detailed results of various magneto-transport behavior will be discussed.


1Supported in part by NSF, DOE and OSU IMR.

4:18PM T20.00006 Tuning the ionization energy of organic semiconductor films: The role of intramolecular polar bonds

NORBERT KOCH, Humboldt-Universitaet zu Berlin — While an isolated individual molecule has only one ionization energy (IE), multiple values are found for molecules in ordered assemblies. Photoelectron spectroscopy of archetypical conjugated organic compounds combined with first-principles calculations and electrostatic modeling reveal the existence of a surface dipole built into molecular layers. Its origin lies in intramolecular polar bonds (IPBs) of the individual molecules, and its magnitude depends on the orientation of molecules relative to the surface of an ordered assembly. Suitable pre-patternning of substrates to induce specific molecular orientations in subsequently grown films thus permits adjusting the IE of one molecular species over up to 1 eV via control over layer morphology. Furthermore, mixing of differently terminated molecules (different IPBs) on a molecular length scale allows continuously tuning the IE of thin organic films between the limiting values of the two pure materials. Surface engineering of organic semiconductors via adjusting the polarity of intra-molecular bonds represents thus a viable alternative for controlling the energetics at organic/(in)organic interfaces.

4:54PM T20.00007 ABSTRACT WITHDRAWN —
5:06PM T20.00008 Perpendicular interaction between donor and acceptor molecules on Au(111) , U.G.E. PERERA, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701 USA, R. MISHIMA, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka 560-8531, Japan, 5-WAJ. HLA, Department of Physics and Astronomy, Ohio University, Athens, OH 45701. — The capability to modify the electronic properties of materials by the interaction between donor and acceptor molecules plays a significant role in molecular electronics. Formation of molecular charge transfer complexes have been observed for different donor acceptor system in a lateral configuration. Here, we present the structural and electronic properties of decamethylmanganocene (Mn(C5Me5)2) and 7,7,8,8-tetracyanoquinodimethane (TCNQ) molecules on a Au(111) surface at 4.6K using low temperature scanning tunneling microscopy (STM) to investigate the perpendicular interaction between the molecules. The molecular complexes were formed by depositing Mn(C5Me5)2 onto predeposited TCNQ on Au(111). The TCNQ formed a well ordered self-assembled clusters on Au(111) and Mn(C5Me5)2 adsorbed either on TCNQ layer or on bare Au(111) surface. Perpendicular interaction between the Mn(C5Me5)2 and TCNQ were determined by means of conductance tunneling spectroscopy. This work provides an important step for manipulating and tuning charge state of molecules using donor-acceptor molecular systems. The research is supported by United States Department of Energy BES grant number DE-FG02-02ER46012.

Wednesday, March 18, 2009 2:30PM - 4:54PM
Session T21 DCMP: Semiconductors: Mechanical and Dynamic Properties 323

2:30PM T21.00001 3D X-Ray Microscopy and Dislocation Dynamics Simulation Investigation of Deformation in Copper1, B. C. LARSON, ORNL, JIE DENG, ANTER EL-AZAB, FSU, J. Z. TISCHLER, ORNL. — We have combined submicron resolution 3D x-ray microscopy measurements at the Advanced Photon Source and discrete dislocation dynamics (DD) simulations to initiate fundamental investigations of deformation in metals. Half-micron resolution 3D x-ray microscopy measurements of local plastic rotation deformation were performed on initially dislocation free Cu single crystals that were compression deformed axially along [100] to strains varying from 1% to 7.6%. Accordingly, dislocation dynamics simulations of axial [100] deformation in fcc Cu were performed for strains ranging up to 1.6%. The overlapping range of the measured and simulated strain magnitudes provides the first direct and quantitative link on mesoscopic length scales between first principles simulations of deformation and submicron resolution deformation measurements. Quantitative comparisons between the measured and simulated local lattice curvatures will be presented in graphical and statistical form.

1Research supported by the US DOE Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering; the APS is supported by the DOE Office of Science.

2:42PM T21.00002 Low speed fracture instabilities in a brittle crystal, NOAM BERNSTEIN, JAMES R. KERMODE, TRISTAN ALBARET, DOV SHERMAN, PETER GUMBSCH, MICHAEL C. PAYNE, GÁBOR CSÁNYI, ALESSANDRO DE VITA. — Brittle materials under mechanical load fail by nucleation and propagation of cracks, and these cracks show well known instabilities at high crack speeds. In this work we show that new instabilities caused by the atomic structure of the crack tip can occur at low crack speeds as well [1]. Using state of the art computer simulations, we find atomic rearrangements at a silicon crack tip on the [111] cleavage plane that occur preferentially on one side of the crack, but only at low crack speeds. Experiments using a novel technique for applying low tensile loads show that real silicon cracks form distinctive features on one side of the exposed crack surface. A mesoscopic model explains how the microscopic atomic rearrangements lead to the observed macroscopic features. We present extensive results on silicon and preliminary results on other brittle materials including sapphire, diamond, and silicon carbide. We conclude that even very brittle single-crystal materials can have a complex crack tip atomic structure, and that atomic scale rearrangements can lead to macroscopic changes in crack morphology. [1] J. R. Kermode et al., Nature 455, 1224 (2008).

2:54PM T21.00003 Thermoelectric damping in micromechanical resonators1, THOMAS METCALF, BRADFORD PATE, DOUGLAS PHOTIADIS, BRIAN HOUSTON, Naval Research Laboratory. — The performance of micro- and nano-mechanical resonators as sensors, filters, and in other devices is determined by the quality factor, Q, which measures the fractional energy loss per oscillation cycle of the resonator. In any given resonator, several energy loss mechanisms are likely to be simultaneously present. However, for micro- and nano-scale resonators, the relative strengths and identity of these mechanisms is largely unknown. We measure the temperature dependence of Q−1 of two resonant modes (460 kHz and 510 kHz) of a 1.5 μm thick silicon micromechanical plate resonator. In-situ ultra-high vacuum annealing lowers the background energy loss at 120 K to Q−1 ≤ 5 × 10−7. The Q−1 increases with increasing temperature by different rates for the two modes, quantitatively agreeing with a modification of Zener’s theory of thermoelastic damping. This provides strong evidence that thermoelasticity is the dominant energy loss mechanism in one resonant mode.

1Work supported by the Office of Naval Research.

3:06PM T20.00004 Ab initio guided design of bcc Mg-Li alloys for ultra light-weight applications , MARTIN FRIÄK, WILLIAM ART COUNTS, DIERK RAABE, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Duesseldorf, Germany. — Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In this paper, fundamental physical properties like formation energies and elastic constants of 11 bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are then used to calculate engineering parameters like (i) specific Young’s modulus (Y/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. The engineering parameters are then used to identify alloys that have optimal mechanical properties needed for a light weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. The specific modulus for alloys with 70 at.% Mg is equal to that of Al-Mg alloys. An Ashby map containing Y/ρ vs. B/G shows that it is not possible to increase both Y/ρ and B/G by changing only the composition or local order of a binary alloy (W. A. Counts, M. Friak, D. Raabe and J. Neugebauer, Acta Mater 57 (2009) 69-76).
3:18PM T21.00005 Thermal Stability of Shape Transition in Strained Nano-Islands. CRISTIANO NISOLI, Los Alamos National Laboratory, DOUGLAS ABRAHAMS, Oxford University, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National Laboratory — Two dimensional Stranski-Krastanow strained islands are known to undergo a shape anisotropy transition as they grow in size, finally evolving toward nanowires. We investigate thermal stability of this process and find a phase transition both in temperature and, in simple cases, in growth. While our results are general, they can explain recent data on Erbium Silicide growth on vicinal Si surface.

3:30PM T21.00006 Neutron Time of Flight phonon spectra of Cu$_2$O and Ag$_2$O powders. BARRY WINN, Brookhaven National Laboratory, MARK HAGEN, Oak Ridge National Laboratory, STEVE SHAPIRO, Brookhaven National Laboratory — Negative thermal expansion materials cuprite (Cu$_2$O) and Ag$_2$O share the same structure (space group Pn3m). Here, we report inelastic neutron time of flight measurements of room temperature powder samples of each system, using the Pharoas chopper spectrometer at LANSCE, at up to 100 meV energy transfer. For Cu$_2$O, high energy optical phonons are observed between 60 and 80 meV, while for Ag$_2$O, these phonons are observed between 50 and 70 meV. Results are compared to previous work, and to recent neutron triple axis spectrometer results for Cu$_2$O, and their relevance to negative thermal expansion is discussed.

3:42PM T21.00007 Large-Amplitude Anharmonic Decay of Coherent A1g phonon motion in Bismuth. STEPHEN FAHY, AARON HURLIE, DONAL O DONOHUE, University College Cork, EAMONN MURRAY, Rutgers University, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, TADASHI OGITSU, Lawrence Livermore National Laboratory, DAVID REIS, University of Michigan, DAVID FRITZ, SLAC, Stanford University — Large amplitude coherent motion of the A1g phonon in bismuth can be generated by ultrafast optical excitation. At low amplitude, the decay rate agrees with that observed in Raman scattering. At high levels of photoexcitation, the observed phonon damping is substantially increased, compared to low-amplitude motion. We present a classical simulation of the anharmonic decay of the phonon, including third-order anharmonic terms in the energy, calculated using density functional perturbation theory, coupling the A1g motion to modes throughout the Brillouin Zone. At low amplitude, the classical decay can be shown in perturbation theory to be almost identical in classical and quantum dynamics at room temperature, demonstrating the validity of a classical simulation of the dynamics. For very large A1g amplitude, the amplitude of motion in the final state modes is substantially increased over their thermal average values, leading to an increase in the decay rate of the A1g mode.

3:54PM T21.00008 Phonon dispersion relations for unstrained Si$_{1-x}$Ge$_x$ via density functional theory. MD HOSSAIN, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA, JONATHAN FREUND, HARLEY JOHNSTON, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA — Phonon dispersions for the Si$_{1-x}$Ge$_x$ alloy system are computed using localized basis density functional theory. Including interactions up to third-nearest-neighbors and the effect of atomic randomness, phonon dispersion for the full Brillouin zone of a supercell containing 8 atoms is computed for 8 different compositions. Frequencies are found to be in excellent agreement with available experimental results for both crystalline Si and Ge. Results are compared with a 64-atom supercell calculation for optical frequencies to show any possible effect of supercell size on the phonon calculation. The atoms in the calculation are relaxed to a force tolerance of 0.0001eV/Å, which is found to be important to correctly determine the dispersion near the Γ- and X-points of the Brillouin zone where q-convergence is harder to achieve. The highest optical phonon frequencies are observed to vary nonlinearly with composition, a fact not investigated before using computational methods.

4:06PM T21.00009 Grating-Enhanced Response for current-driven coupled quantum wells¹. ANTONIOS BALASSIS, Fordham University, GODFREY GUMBS, Hunter College/CUNY — We have investigated the conditions necessary to achieve stronger plasmon instability leading to emission in the terahertz (THz) regime for semiconductor quantum wells (QWs). The surface response function is calculated for a bilayer two-dimensional electron gas (2DEG) system in the presence of a metal grating placed on the surface and which modulates the electron density. The 2DEG layers are coupled to surface plasmons arising from excitations of free carriers in the bulk region between the layers. A current is passed through one of the layers and is characterized by a drift velocity $v_D$. With the use of the surface response function, the plasmon dispersion equation is obtained as a function of frequency $\omega$, the in-plane wave vector $q_{\parallel} = (q_x,q_y)$ and reciprocal lattice vector $G$ where $n = 0, \pm 1, \pm 2, \cdots$ and $G = 2\pi/n$ with $d$ denoting the period of the grating. The dispersion equation, which yields the resonant frequencies, is solved in the complex plane for real wave vector $q_{\parallel}$. It is ascertained that the imaginary part of $\omega$ is enhanced with decreasing $d$, and with increasing the doping density of the free carriers in the bulk medium for fixed grating period.

¹Supported by contract FA 9453-07-C-0207 of AFRL.

4:18PM T21.00010 Where the reactive sites are in anatase nanoparticles? — Theoretical Investigations on (001) and (101) surfaces in anatase nanoparticles. HONG WANG, JAMES LEWIS, West Virginia University — Recently, with the development of nanotechnology, the devices’ size shrinks to nano-scale size where the surface properties play a role. Thus, it is required scientists to provide fundamental level understanding of anatase surfaces in nano-size anatase materials to improve its applications. In this work, applying DFT ab initio method, we investigate the fundamental properties of anatase (001) and (101) surfaces in anatase nanoparticles. By adopting different portions of (001) and (101) surfaces along with the size of nanoparticles, we analyze the geometric properties and energetic stabilities of nanoparticles. The electronic properties of these nanoparticles are also calculated in this work. The frontier orbitals located mostly in the (001) surfaces indicate these sizes are possibly reactive sizes in the external molecular adsorption reaction. To verify their activity, we add water molecules in different sites and different concentration on these nanoparticles. The results show that the sites where the frontier orbitals are localizing are very reactive for water adsorption.

4:30PM T21.00011 Collective Excitations in Cylindrical Quantum Dots Chains. JIMENA VERGARA, ANGELA CAMACHO, Universidad de los Andes — We are interested in the study of collective excitations in quantum dot chains because these can be used to effectively transmit information at nano scale and to control spontaneous and stimulate electromagnetic emission in the quantum dots. [1] This work is centered in the study of semiconductor one-dimensional quantum dot arrays. Based on a tight-binding bandstructure calculation combined with a self consistent field approximation we obtain the dispersion relations and we analyze how the geometry of the dot affects the collective oscillation of charge and its propagation. We focus our study first on Coulomb interaction between charges as the main cause of the 1D plasmons neglecting tunneling to finally compare with the case where tunneling is allowed. We find out that Coulomb interaction plays an important role in these systems and that tunneling opens the energy spectrum permitting new excitations, which are good candidates to be used in nanometric devices. [1] A.V.Akimov, A.Mukherjee, C.L. Yu, D.E Chang, A.S.Zybrov, P.R. Hemmer, H Park and M.D Lukin, *Generation of Single optical plasmons in metallic nanowires coupled to quantum dots*, Nature 450, 402 (2007).
4:42PM T21.00012 Electrical characterization of MOVPE-grown InSb nanowires, HENRIK NILSSON, PHILIPPE CAROFF, CLAES THELANDER, MARCUS LARSSON, LARS-ERIK WERNERSSON, LARS SAMUELSON, HONGQI XU, SOLID STATE PHYSICS TEAM — In bulk, InSb is a narrow band gap ($E_g = 170$ meV) semiconductor with high electron mobility ($\mu = 77000 \text{ cm}^2/\text{Vs}$) and is therefore of relevance for low power and high speed circuit applications. It also has a low electron effective mass ($m_\text{e} = 0.015 m_0$) and a very high electron g-factor ($|g| = 51$) which is of interest for studies of quantum and spin physics. InSb nanowires were grown by MOVPE from 40 nm Au aerosol seed particles deposited on a $<111>$ B InAs substrate, where the growth was initiated by a 100 nm InAs segment. The InSb nanowires are untapered and free from stacking faults. The grown InSb nanowires were transferred to degenerately doped, SiO$_2$ capped, Si substrates. After locating the wires, Ti/Au contacts were made by electron beam lithography. Electrical measurements of the fabricated InSb nanowire devices were performed in the high bias, field-effect transistor (FET) regime at temperatures ranging from 300 K to 4.2 K as well as in the low bias, single-electron transistor (SET) regime at temperatures ranging from 4.2 K to 300 mK. In particular, effective electron g-factors and Kondo physics have been studied at low temperatures with the nanowire devices.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T22 GMAG DMP FIAP: Focus Session: GaMnAs 324

2:30PM T22.00001 Electric-field manipulation of magnetization vector direction\(^1\), HIDEO OHNO, RIEC, Tohoku University / ERATO JST — Ferromagnetism and magnetization in Mn-doped III-V semiconductors can be manipulated by various means; by changing its carrier concentration by electric fields \([1]\) or by spin-current flowing along with the electric current \([2]\). This material system is thus an excellent system to study the physics involved in manipulation of magnetism as well as exploring new ways to control magnetization. Here, we show that electrical control of magnetization direction can be done through manipulating electronically the magnetic anisotropy energies \([3]\). The basic idea behind the effort is to control the population of carriers on spin-split anisotropic valence bands that governs the magnetic anisotropy energies, which should result in change of the direction of magnetization. In order to measure the magnetic anisotropy under a gate that applies the electric-field to the ferromagnetic semiconductor channel, we used the planar Hall effect. Analyses showed that there are biaxial as well as unaxial anisotropies. As the sheet carrier concentration is reduced by applying electric-field to the channel, the uniaxial anisotropy field reduced its magnitude and eventually changed its sign, whereas no significant change was apparent in the biaxial anisotropy field. From the electric-field dependent anisotropy fields, one can show that the angle of the magnetization direction in the absence of magnetic fields is modified by electric-fields by 10 degrees. This opens up a new and unique opportunity for manipulating magnetization direction solely by electronic means, not resorting to magnetic-field, spin-current, mechanical stress, nor multiferroics. The conditions for switching the magnetization direction will also be discussed. The work was done together with D. Chiba, F. Matsukura, M. Sawicki, Y. Nishitani, and Y. Nakatani.


\(^1\)The word was supported in part by the “Research and Development for Next-Generation Information Technology” program from MEXT, Japan.

3:06PM T22.00002 Bias-controlled ferromagnetism in quantum wells with Mn-delta doping, ERIKA DIAS CABRAL, SUNY Buffalo and UERJ, Brazil, RAFAEL OSZWALDOWSKI, SUNY Buffalo and N. Copernicus University, Torun, Poland, MARCO BOSELLI, IGOR ZUTIC, SUNY Buffalo, IVAN DA CUNHA LIMA, UERJ, Brazil — Carrier-mediated magnetism in semiconductors shows important and potentially useful differences from magnetism in metals \([1]\) such as light- or bias-controlled ferromagnetism \([2-3]\). Motivated by experiments reporting in GaAs quantum wells (QWs) with Mn-delta doping higher Curie temperatures ($T_C$) than in bulk (Ga,Mn)As \([4]\), we explore theoretically the feasibility of bias-controlled ferromagnetism in QWs. We calculate self-consistently indirect Mn-Mn exchange interaction \([5]\) and apply a Monte Carlo approach to calculate $T_C$. Our approach allows us to systematically study the effects of quantum confinement and the position of the Mn layer on magnetic ordering and $T_C$, beyond the mean field approximation, which we obtain as the limiting case. We compare our findings with the experimental results and suggest paths towards improved control of ferromagnetism. Supported by CNpq, FAPEMIG, FAPEJ, CAPES, US ONR, and NSF-ECCS Career. \[1\] I. Zutic et al., Rev. Mod. Phys. 76, 323 (2004). \[2\] S. Koshihara et al., Phys. Rev. Lett. 78, 4617 (1997). \[3\] H. Ohno et al., Nature 409, 944 (2000). \[4\] A. M. Nazmul et al., Phys. Rev. Lett. 95, 017201 (2005). \[5\] M. A. Boselli et al., Phys. Rev. B 68, 085319 (2003).

3:18PM T22.00003 STM studies of an atomic-scale gate electrode formed by a single charged vacancy in GaAs, DONGHNUG LEE, DAVID DAUGHTON, JAY GUPTA, The Ohio State University — Electric-field control of spin-spin interactions at the atomic level is desirable for the realization of spintronics and spin-based quantum computation. Here we demonstrate the realization of an atomic-scale gate electrode formed by a single charged vacancy on the GaAs(110) surface\([1]\). We can position these vacancies with atomic precision using the tip of a home-built, low temperature STM. Tunneling spectroscopy of single Mn acceptors is used to quantify the electrostatic field as a fraction of distance from the vacancy. Single Mn acceptors are formed by substituting Mn adatoms for Ga atoms in the first layer of the p-GaAs(110) surface\([2]\). Depending on the distance, the in-gap resonance of single Mn acceptors can shift as much as 200meV. Our data indicate that the electrostatic field decays according to a screened Coulomb potential. The charge state of the vacancy can be switched to neutral, as evidenced by the Mn resonance returning to its unperturbed position. Reversible control of the local electric field as well as charged states of defects in semiconductors can open new insights such as realizing an atomic-scale gate control and studying spin-spin interactions in semiconductors. http://www.physics.osu.edu/~$\sim$gupta\[1\] D. Lee and J.A. Gupta (in preparation) \[2\] D. Kitchen et al., Nature 442, 436-439 (2006)

3:30PM T22.00004 Probing the nature of electronic state near the Fermi level in Ga$_{1-x}$Mn$_x$As with STM, ANTHONY RICHERDella, Princeton University / UIUC, PEDRAM ROUSHAN, Princeton University, SHAWN MACK, DAVID AWSCHALOM, UCSB, ALI YAZDANI, Princeton University — We have studied the electronic states near the Fermi energy in GaMnAs/GaAs heterostructures as a function of doping across the metal-insulator transition. These measurements allow us to determine the position of $E_F$ with respect to the valance band edge and in gap states related to the Mn induced acceptor states. As the doping level increases we observe an increase in the density of states at the Fermi energy and map their spatial dependence. Statistical analysis of these measurements can be used to find a characteristic length scale associated with growth of bulk metallic behavior for these samples. In addition, our measurements indicated a suppression of the density of states near $E_F$ at all doping levels, consistent with that expected for correlation effects in doped semiconductors near the metal-insulator transition. We will discuss these findings and their relation with various theoretical models for electronic states in GaMnAs that are expected to mediate the magnetic interaction in this compound.

\(^3\)This work is supported by ARO, ONR, NSF and ASEE.
3:42PM T22.00005 Scanning Tunneling Microscopy Studies of Mn acceptor levels in Ga$_{1-x}$Mn$_x$As

PEDRAM ROUSHAN, ANTHONY RICHARDELLA, Princeton University, SHAWN MACK, DAVID, AWSCHALOM, UCSCB, ALI YAZDANI, Princeton University — We have used a low temperature scanning tunneling microscope (STM) to perform studies of GaMnAs/GaAs heterostructures with various Mn dopant concentrations. The STM topography of the GaMnAs showed a variety of electronic structure modulations on the order of a few nm indicating the presence of a high level of disorder and compensation. These measurements show no indication of Mn clustering as the Mn concentration is increased. On both sides of the Metal-Insulator Transition (MIT), the differential conductance (dI/dV) measurements on Mn dopants showed a broad acceptor level above 100meV from the valence band edge. Furthermore, we have mapped in energy the spatial variations of these deep acceptor levels, and their distribution will be presented for all Mn concentrations studied. The effect of disorder and coulomb correlations in modifying the local density of states close to Fermi level will be discussed for insulating as well as metallic samples.

1This work is supported by ARO, ONR, NSF and ASEE.

3:54PM T22.00006 Theory of STM spectroscopy in Mn clusters on GaAs surfaces.

TOR OLOF STRANDBERG, Lund University, ALAN MACDONALD, University of Texas at Austin, CARLO CANALI, Kalmar University — Small numbers of Mn atoms can be manipulated into arbitrary spatial arrangements on the <110> surface of GaAs by means of a novel STM atom-by-atom substitution technique, which enables the replacement of individual Ga atoms by Mn [1]. The tunneling differential conductance over an isolated Mn atom reveals a broad and large resonance in the GaAs energy gap. For a Mn pair placed less than 1 nm apart, the resonance splits into two peaks, whose spacing is thought to be related to the exchange-energy interaction between Mn ions. We report on theoretical results for the local density of states and the Mn acceptor-level splittings for a Mn dimer, based on a tight-binding model of Mn substitutions on the <110> GaAs surface. We compare our model with previous work which does not account for the surface. We then derive an effective quantum spin Hamiltonian for the Mn cluster, based on a Chern number theory developed recently, which includes Berry phase effects [2]. We study the transition from surface to bulk for the substitutional Mn impurity in GaAs as well as Mn-Mn interactions at the surface and in bulk at various distances and along different crystalline directions. [1] D. Kitchen et al., Nature 442, 436 (2006). [2] C.M. Canali, A. Cehovin and A.H. MacDonald, Phys. Rev. Lett. 91, 046805 (2003)

4:06PM T22.00007 Strong Magnetic Circular Dichroism in Mn Delta-doped GaAs.

NAZMUL AHSAN, SANJUKTA GHOSH, MASAKA TANAKA, University of Tokyo — Delta-doping of magnetic impurities (i.e., Mn) in III-V semiconductors allows locally high concentration of magnetic moments. This can lead to systematic observation of fundamental properties of the system including the enhancement of the Curie temperature and magnetic anisotropy as a function of a wider range of Mn concentration[1]. The delta-doped Mn atoms in the MBE-grown GaAs-based heterostructures are abruptly confined as confirmed by high resolution transmission electron microscopy studies[1]. Here we study the magnetic circular dichroism (MCD) of 1 monolayer (ML) Mn delta-doped GaAs layer. The structure from the growth sequence is: GaAs substrate/GaAs-buffer/Al$_x$Ga$_{1-x}$As/1mn GaAs/1ML Mn/10nm GaAs cap. The sample was chemically etched to single out the 1mn GaAs/1ML Mn layer/10nm GaAs cap to measure MCD spectra in the transmission geometry. We observed strong MCD features even at 300K, indicating ferromagnetism with zinc-blende band structure. Ref.: [1] Nazmul et al. Phys. Rev. B 67, 241308 (2003); J. Crystal Growth, 221, 303 (2003); Phys. Rev. Lett. 95, 017201 (2005); Phys. Rev. B 77, 155203 (2008).


C. SUN, Rice University, J. KONO, Rice University, Y.H. CHO, A.A. BELYANIN, Texas A&M University, H. MUNEKATA, Tokyo Institute of Technology — The role of impurity bands as well as the nature of free holes in carrier-mediated ferromagnetism in (III,Mn)V systems are still not well understood. Previous magneto-optical studies of GaMnAs have produced an array of conflicting results, especially in terms of the nature of optical transitions involved. Here, we have performed systematic magneto-optical Kerr spectroscopy studies of GaMnAs samples with different doping densities. The Kerr angle strongly depended on the photon energy, showing positive peaks at 1.7 eV and 3 eV and a negative peak at 2.5 eV. The 1.7 eV peak clearly shifts to higher energies with Mn doping from 1% to 2.4% and shifts to an even higher energy after annealing. We attribute these changes to the increased hole density and effective Mn content. A 30-band $k$ - p model with exchange interaction is adopted to simulate the spectra. The excellent agreement between the experiment and calculation leads us to conclude that Kerr rotation in GaMnAs above the band gap is dominantly determined by interband transitions.

4:30PM T22.00009 Below band gap Faraday and Kerr measurements in ferromagnetic GaMnAs.

GHEORGHE ACBAS, M.-H. KIM, J. CERNE, Physics Dept. Univ. at Buffalo, SUNY, Buffalo, NY, M. CUJKR, V. NOVAK, T. JUNGWIRTH, Institute of Physics, Acad. of Sciences of the Czech Republic, Prague, Czech Republic, M.A. SCARPULLA, Materials Department, Univ. of California, Santa Barbara, O.D. DUBON, Mat. Sci. & Eng. Dep., Univ. of Poitiers, Berlin, J. SINOVA, Physics Dept., Texas A&M Univ., College Station, TX — We have studied the Faraday and Kerr effects in a series of ferromagnetic GaMnAs films in the 115-1500 meV energy range. This provides a direct magneto-optical probe of the magnetic properties of a continuous (Ga,Mn)As film such as saturation magnetization and anisotropy field. These new approaches to scanned magnetic force imaging open the door to powerful new tools for spatially resolved studies of nanoscale magnetism and spin-based devices.

4:42PM T22.00010 Local Magnetic Characterization of Continuous (Ga,Mn)As Film using Mechanical Force Detection.

J. H. LEE, YU. OBUKHOV, J. KIM, The Ohio State University, X. LI, N. SAMARTH, The Pennsylvania State University, D. V. PELEKHOV, P. C. HAMMEL, The Ohio State University — We report on low temperature (T = 4.2 K) studies of the local spin dynamics in ferromagnetic samples using Ferromagnetic Resonance Force Microscopy (FMRFM) and probe-induced Magnetic Force Microscopy (MFM). Both techniques are based on sensitive mechanical detection of the dipolar magnetic interaction between a micromagnetic probe mounted on a flexible micro-cantilever and magnetic moments in the sample. The probe magnet not only detects the magnetic force, but also perturbs sample spin magnetization by adding the strongly inhomogeneous magnetic field. We demonstrate that the combination of FMRFM and probe-induced MFM can be used to extract and map local magnetic properties of a continuous (Ga,Mn)As film such as saturation magnetization and anisotropy field. These new approaches to scanned magnetic force imaging open the door to powerful new tools for spatially resolved studies of nanoscale magnetism and spin-based devices.

3This work was supported by the U.S. Department of Energy through Grant No. DE-FG02-03ER46054
4:54PM T22.00011 Simultaneous Optical Imaging and Electrical Control of Magnetization in (Ga,Mn)As

M.E. NOWAKOWSKI, G.D. FUCHS, D.D. AWSCHALOM, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106, A. BALK, M.J. WILSON, N. SAMARTH, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, PA 16802 — Spin dependent phenomena in metals and semiconductors promises the development of low-power logic and memory devices based on electrical control of the magnetization. To realize this potential, precise visual information of magnetic domains is required to design and control electrical structures manipulated by the spin transfer torque. We present studies of magnetization behavior in micron-scale (Ga,Mn)As channels using a recently developed video-rate magneto-optical Kerr effect microscope. Measurements record real-time, diffraction-limited, surface magnetization information including magnetic switching and domain wall motion. The optical measurements are correlated with simultaneous electrical measurements to provide insight into pinning and magnetization transport in these structures.

1Work supported by ONR

5:06PM T22.00012 Optical conductivity of diluted magnetic semiconductors: effects of dynamical screening1 , FEDIR KYRYCHENKO, CARSTEN A. ULLRICH, University of Missouri — Most theoretical studies of transport and optical conductivity in diluted magnetic semiconductors like GaMnAs treat disorder and many-body effects within the simple relaxation time and static screening models. Here we present a more complete theory of transport in charge and spin disordered media that combines a multiband k · p approach with a first-principles descriptions of disorder and electron-electron interaction through the memory function formalism and time-dependent density functional theory. We discuss the effects of dynamic screening and collective electron excitations on the charge and spin scattering off Coulomb impurities and fluctuations of localized spins and compare calculated values of optical conductivity in GaMnAs with experimental results.

1This work was supported by DOE grant DE-FG02-05ER46213.

5:18PM T22.00013 Infrared probe of Ga1−xMnxAs films with controlled disorder and compensation , BRIAN CHAPLER, University of California San Diego, R.C. MYERS, Ohio State University, S. MACK, D.D. AWSCHALOM, University of California Santa Barbara, M.C. MARTIN, Lawrence Berkeley National Laboratories, A. DATTELBAUM, Los Alamos National Laboratory, K.S. BURCH, University of Toronto, D.N. BASOV, University of California San Diego — Arsenic antisite defects (AsGa) formed due to low temperature growth conditions are a leading cause of disorder and compensation in Ga1−xMnxAs. Samples grown with gradient As:Ga growth condition for 0.005 < x < 0.16 have allowed for optimized As flux minimizing AsGa. By studying samples at this optimized location via infrared spectroscopy, a new level of precision can be attained in exploring the electronic structure and other intrinsic properties of Ga1−xMnxAs samples. Using optical sum rule analysis of our experimentally determined optical conductivity (σf(ω)), we extract the free carrier band mass (m*) and find it to be several m0. We also comment on the levels of interstitial Mn (Mn2-), finding for x > 0.03 roughly 25% of Mn resides at an interstitial location. Additionally, by probing positions along the As:Ga gradient we directly measure the effects of disorder and compensation on these samples. Systematic changes in σf(ω) as AsGa content is increased are reported, and the consequences of this on our understanding of the electronic structure of Ga1−xMnxAs are discussed.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T23 DCMP FIAP: Quantum Hall Effect: Coherent Phenomena 325

2:30PM T23.00001 Low-field quantum Hall transport in an electron Fabry-Perot interferometer , P.V. LIN, F.E. CAMINO1, V.J. GOLDMAN, Stony Brook University — We report systematic experimental characterization of an interferometer device as a function of front-gate voltage at 10 mK. Application of front-gate voltage affects the constriction electron density, but the 2D bulk density remains unaffected. The low-field quantum Hall transport (filling f > 4) shows quantized plateaus in longitudinal resistance, while the Hall resistance is dominated by the low-density, low-filling constriction. This allows to determine independently both: the bulk and the constriction filling. At lower fields, when the quantum Hall plateaus fail to develop, we observe the bulk Shubnikov-de Haas oscillations in series corresponding to an integer number of the magnetoelectric subbands in the conduction. From a Fock-Darwin analysis, we obtain the constriction electron density as a function of the front-gate bias, and, extrapolating to the zero-field, the B = 0 number of 1D electric subbands (conductance channels) resulting from the electron confinement in the constriction.

1Present address: Center for Functional Nanomaterials, Brookhaven National Laboratory

2:42PM T23.00002 Oscillatory transport in electron Fabry-Perot interferometers , F.E. CAMINO1, P.V. LIN, V.J. GOLDMAN, Stony Brook University — We report experiments on GaAs/AlGaAs heterostructure interferometers in the integer QH regime with filling f = 1 − 4. Etch trenches define the device, which consists of an electron island connected to the 2DES bulk via two wide constrictions. Front gates deposited in the trenches permit to fine tune the device. When tunneling occurs in the constriction, electrons perform closed orbits around the island, producing an Aharonov-Bohm oscillatory signal in the conductance. On QH plateau transition between f + 1 and f, we observe f oscillations per flux h/e. In contrast, for all fillings, we observe one oscillation per back-gate charging period ε. We also report a linear dependence of magnetic field period on front-gate voltage for three devices, with the slope inversely proportional to f. We attribute this behavior to self-consistent electrostatics of the electron island, and discuss the models of edge channel structure.

1Present address: Center for Functional Nanomaterials, Brookhaven National Laboratory

2:54PM T23.00003 Universal dephasing in chiral one-dimensional electron systems , FLORIAN MARQUARDT, CLEMENS NEUENHAHN, Arnold Sommerfelld Center for Theoretical Physics, Center for NanoScience, and Department of Physics, Ludwig-Maximilians University Munich — The Green’s function of a chiral interacting one-dimensional fermion system obeys a power-law decay at high energies, at zero temperature. Surprisingly, we find that the exponent is universal, i.e. independent of the interaction strength, for (almost) arbitrarily shaped interaction potentials. This has direct implications for the interference contrast in ballistic interferometers, e.g. the Mach-Zehnder interferometer composed of edge channels in the integer quantum Hall effect. Our result is obtained using a straightforward and physically transparent “semiclassical” approach to dephasing by electron-electron interactions. This approach is shown to coincide with the exact bosonization results in the high-energy regime of interest.
3:06PM T23.00004 Determination of the coherence length in the Integer Quantum Hall Regime. F. PORTIER, P. ROULLEAU, P. ROCHE, CEA Saclay, SPEC, Nanoelectronic group, F-91919 Gif-sur-Yvette, A. CAVANNA, G. FAINI, U. GENSIBER, D. MAILLY, CNRS, LPN, Phynano team, Route de Nozay, F-91400 Marcoussis, NANOELECTRONIC GROUP COLLABORATION, PHYNANO TEAM COLLABORATION — One of the basic length scales limiting quantum effects in electrical conductors is the phase coherence length Lϕ, the typical length on which an excitation loses its phase coherence via coupling to other degrees of freedom. In quasi-1D diffusive wires, due to electron-electron interactions, Lϕ was shown to scale as T−1/3 as predicted by Altshuler-Aronov-Khmelnitsky. Surprisingly, little is known about Lϕ in the Integer Quantum Hall Regime (IQHE), where transport occurs through 1D chiral wires, localized on the edges of the sample. The number of these ‘edge states’ is equal to the filling factor (the number of electron per flux quantum flux). Chirality should prevent momentum conserving energy exchange processes, leading to a very long coherence length. We present an experiment where we have determined Lϕ in the IQHE at filling factor 2, by measuring the visibility of quantum interferences in an electronic Mach-Zender interferometer. Lϕ shows a T−1 dependence, proved to result from the coupling between the two neighbouring edge states: the thermal charge noise in one edge state blurs the phase on the other edge state, leading to a finite coherence length proportional to T−1.

3:18PM T23.00005 Edge-State Velocity and Coherence in a Quantum Hall Fabry-Perot Interferometer1. DOUGLAS MCCLURE, YIMING ZHANG, ELI LEVENSON-FALK, CHARLES MARCUS, Harvard University, LOREN PFIEFFER, KEN WEST, Bell Labs, Alcatel-Lucent — We present finite-bias measurements of electronic Fabry-Perot interferometers in the integer quantum Hall regime. In devices large enough that Coulomb blockade is absent, checkerboard-like patterns of oscillations as a function of magnetic field and dc bias appear. Comparing our data to predictions for electromagnetic Aharonov-Bohm interference, we extract edge-state velocities over a range of magnetic fields, finding dependence consistent with a crossover from skipping orbits at low fields to E x B drift at high fields. Suppression of visibility observed at high bias and high field is quantitatively accounted for by including an energy-dependent dephasing rate.

3:30PM T23.00006 Distinct Signatures For Coulomb Blockade and Aharonov-Bohm Interference in Electronic Fabry-Perot Interferometers1. YIMING ZHANG, DOUGLAS MCCLURE, ELI LEVENSON-FALK, CHARLES MARCUS, Harvard University, LOREN PFIEFFER, KEN WEST, Bell Labs, Alcatel-Lucent — We present finite-bias measurements of electronic Fabry-Perot interferometers of different sizes. Measuring these oscillations as a function of magnetic field, gate voltage, or both, we observe three signatures that distinguish the two types. The oscillations observed in a 2 µm² device are understood to arise from Coulomb blockade, and those observed in an 18 µm² device from Aharonov-Bohm interference. This work clarifies, provides ways to distinguish, and demonstrates control over, the physical origins of resistance oscillations seen in electronic Fabry-Perot interferometers.

3:42PM T23.00007 Fabry-Perot interferometer in Fractional Quantum Hall regime. AVEEK BID, N. OFEK, M. HEIBLUM, ADY STERN, V. UMANSKY, D. MAHALU, Weizmann Institute of Science — We have measured Aharonov-Bohm/Coulomb blockade oscillations in an electronic Fabry-Perot interferometer in the Fractional Quantum Hall regime. At ν = 2/5, when the inner channel is partially reflected (with the outer channel (1/3) being fully transmitted); the total transmission of the device oscillates as a function of magnetic field or modulation gate voltage. This is true also for ν = 2, 3, 4 when the interference is of a partially reflected lower lying channel (with the other channels being either fully transmitted or fully reflected). However, in the outermost channel of all filling factors (ν = 1/3, 2/5, 1, 4/3, 2, 3, 4, 5) we do not see any oscillations as a function of B. This we interpret to be due to interplay between the magnetic field (which tries to modify the area of the compressible island inside the interferometer) and Coulomb energy (which prevents the density of quasiparticles within the island from building up indefinitely). The period of oscillations in modulation gate voltage in the inner channel of ν = 2/5 (partially partitioned) is found to be one-third of that observed in the second channels of the integer filling fractions which probably is an indication that the oscillations are due to the tunnelling of quasiparticles of fractional charge 1/3.

3:54PM T23.00008 Nonequilibrium Dephasing in an Electronic Mach-Zehnder Interferometer. SEOK-CHAN YOUN, KAISS, HYUN-WOO LEE, POSTECH, H.-S. SIM, KAISS — We study nonequilibrium dephasing in an electronic Mach-Zehnder interferometer. We demonstrate that the shot noise at the beam splitter of the interferometer generates an ensemble of nonequilibrium electron density configurations and that electron interactions induce configuration-specific phase shifts of an interfering electron. The resulting dephasing exhibits two characteristic features, a lobe pattern in the visibility and phase jumps of π, in good agreement with experimental data.

4:06PM T23.00009 Generating Excitonic Supercurrent in Quantum Hall Bilayers. JUNG-JUNG SU, University of Texas at Austin, TAMIR PEREG-BARNÉA, Physics Department, California Institute of Technology, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin — Among the many examples of Bose condensation considered in physics, exciton condensation has maintained special interest because of controversy about condensate properties. Although ideal condensates can support an exciton supercurrent, it has not been clear how such a current could be induced or detected. We discuss the circuit conditions required to induce a steady-state counterflow superfluid. In addition, we will discuss interpretations of tunnel, drag and counterflow experiments in quantum Hall exciton condensates.

4:18PM T23.00010 Density imbalance effect on the Coulomb drag upturn in an undoped electron-hole bilayer. CHRISTIAN MORATH, JOHN SEAMONS, JOHN RENO, MIKE LILLY, Sandia National Lab — A low-temperature upturn of the Coulomb drag resistivity measured in an undoped electron-hole bilayer (uEHBL) device, possibly manifesting from exciton formation or condensation, was recently observed. The effects of density imbalance on this upturn are examined. Measurements of drag as a function of temperature in a uEHBL with a 20 nm wide Al0.05Ga0.95As barrier layer at various density imbalances n/p are presented. The results show drag increasing as the density of either two dimensional system was reduced, both within and above the upturn temperature regime and with a significantly stronger dependence than the (np)^−3/2 predicted by the weak-coupling theory. A comparison of the data with numerical calculations of drag in the presence of electron-hole pairing fluctuations, which qualitatively reproduce the drag upturn behavior and easily accommodates density imbalance effects, is also presented. The calculations predict a peak in drag at matched densities, which is consistent with the experiments. This work was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.
material. Bi-dislocation lines are associated with one-dimensional fermionic excitations in a 'topological insulator', a novel band insulator believed to be realized in the bulk to propagating fermion modes. Can analogous phenomena occur in crystalline solids that host a plethora of topological defects? Here we show that indeed systems like the B-phase of superfluid helium He.

VISHWANATH, UC Berkeley — Topological defects, such as domain walls and vortices, have long fascinated physicists. A novel twist is added in quantum respecting the discrete symmetries of the system. We construct a tight-binding model on the diamond lattice that realizes the topologically nontrivial phase the topological properties of this quantum state manifest themselves through gapless surface states, that are robust against localization from random impurities transport in topological insulators. Our results provide a novel route to creating a potentially ideal quantum wire in a bulk solid.

quantum spin-Hall insulator, and not scattered by disorder. Since dislocations are ubiquitous in real materials, these excitations could dominate spin and charge rates on the excitation energy and intensity, spin-orbit interaction and a detailed understanding of the role of active phonon modes.

Our ab initio studies directly mimic the experimental data and reveal many intriguing features of the excitation dynamics, including non-radiative fluorescence, fast intrinsic intraband relaxation, phonon-induced component of fluorescence linewidths, the importance of defects, the dependence of the relaxation time-dependent density functional theory in order to model the ultrafast photoinduced processes in carbon nanostructures at the atomistic level and in real time. and even a superconductivity mechanism. We have developed state-of-the-art non-adiabatic molecular dynamics techniques and implemented them withinlinked to the topology of the electronic states of the bulk. The edge modes can be easily investigated when the edges are smooth and have a periodicity, but as soon as the periodicity is absent, the problem becomes un-traceable by purely theoretical means. In my talk I will exemplify the use of non-commutative calculus to explore the properties, especially the stability of the edge modes. For example, using such techniques one can give a fairly elementary proof that the edge modes in Chern insulators survive even for a rough (random) edge. Similarly, for the Spin-Hall effect, one can define an observable and its associated current whose conductance remains quantized during various deformations of the Hamiltonian system. It turns out that in all cases, the edge conductance is given by the index of a Fredholm operator, which provides a new topological invariant linked directly to the edge rather than the bulk.

This research was supported by an award from Research Corporation for Science Advancement.
SWNTs with diameters


Exciton Distribution between the Bright and Dark States in Single Carbon Nanotubes Studied by Magneto-Photoluminescence Spectroscopy , RYUSUKE MATSUNAGA, KAZUNARI MATSUDA, YOSHIHIKO KANEMITSU, Institute for Chemical Research, Kyoto University — We have performed micro-photoluminescence (PL) spectroscopy for single carbon nanotubes under magnetic fields at various temperatures. Sharp PL spectra of single carbon nanotubes allow us to directly observe the bright exciton PL peak a few meV below the bright exciton PL peak due to the Aharonov-Bohm effect [1]. From the PL intensity ratio of the dark to the bright exciton PL in a (6,5) nanotube and concluded they could be used to energetically locate the K-momentum excitons (Torrens, et al, PRL 101, 157401 (2008)). Here we use a combination of experiment and theory to study X\textsc{1} and X\textsc{2} in at least ten samples that are highly purified in a single chirality and use these findings to study how the K-momentum exciton energy depends on chirality.

This work supported by NSF MRSEC DMR-0520020.

Exciton Radiative Lifetimes and Their Temperature Dependence in Single-Walled Carbon Nanotubes , , LAIN-JONG LI, FUMING CHEN, Nanyang Technological University, MINGLI JIA, Chinese Academy of Sciences, LI WEI, YUAN CHEN, M. B. CHAN-PARK, Nanyang Technological University, ANDONG XIA, Chinese Academy of Sciences — The optimal excitation wavelength for the energy transfer from aromatic polymers poly(9,9-dioctylfluorene-2,7-diyl) (PFO) to single-walled carbon nanotubes (SWNTs) is tunable in a wide wavelength range (from 388 to 480 nm) depending on the concentration of excess PFO polymers. The concentration governs the aggregation state and chain conformation of the polymers proximate to SWNT surfaces, which in turn alters the optical excitation wavelength. This study suggests an exciting and convenient method of adjusting the desired optical wavelengths for the energy conversion, useful for polymer-SWNT composites in optoelectronic applications.

Effects of Exciton-Exciton Annihilation in Fluorescence of Individual SWCNTs , ANNI SIITONEN1, SERGEI BACHILO, DMITRI TSYBOULSKI, R. BRUCE WEISMAN, Rice University — Most studies of SWCNT exciton relaxation have been performed on bulk samples, with clear conclusions hampered by the variety of structural types, lengths, and aggregation states. To avoid such problems, we use near-IR fluorescence microscopy to study nearly pristine individual nanotubes with optically resolvable lengths. We find emission proportional to excitation at low intensities. But for stronger excitation, an increasingly sub-linear dependence is observed, due to exciton-exciton annihilation within single nanotubes. Since annihilation depends on excitation lifetime and mobility, these parameters can be studied by analyzing measured intensity dependences. We compare data on exciton excitation ranges and emission efficiency in individual SWCNTs to numerical simulations to quantify exciton lifetime and diffusion for a variety of (n,m) structures. Preliminary results yield lifetimes of a few nanoseconds for nearly pristine, highly emissive nanotubes and reveal some dependence of lifetime on nanotube diameter.

1University of Jyvaskyla

Exciton Spectroscopy and Absorption Cross-section of Individual Single-Walled Carbon Nanotubes . LAURENT COGNET, Bordeaux University and CNRS, France — Semiconducting Single-Walled Carbon Nanotubes (SWNTs) display intrinsic exciton luminescence which is highly sensitive to the nanotubes environment. For instance single-molecule chemical reactions with individual SWNTs could be observed through the stepwise changes of the luminescence intensity within submicrometer segments of single nanotubes. Analysis of the step amplitudes revealed an exciton diffusion range of ~90 nm. Each exciton thus visits approximately 10^3 atomic sites during its lifetime, providing highly efficient sensing of local chemical and physical perturbations [1]. SWNT luminescence decays are also sensitive to extrinsic factors. Using highly luminescent individual (6,5) SWNTs, time-resolved spectroscopy revealed however systematic biexponential luminescence decays, with short and long lifetimes around 45 and 250 ps. This intrinsic behavior is attributed to the band-edge exciton fine structure with a dark level lying a few meV below a bright one. Combining such time-resolved studies with cw luminescence ones, the absorption cross-section of individual SWNTs was determined. A mean value of ~10^17 cm^2 per carbon atom is obtained for (6,5) tubes excited at their second optical transition [2]. This was further corroborated by independent photothermal heterodyne measurements. Because this highly sensitive method relies only on light absorption, it readily detects metallic nanotubes as well as the emissive semiconducting species in various environments and allowed recording for the first time images and absorption spectra of individual SWNTs of both types [3].


Controlling Optimal Excitation Wavelength of Energy Transfer from Photo-Excited Polymers to Single-Walled Carbon Nanotubes. , LAIN-JONG LI, FUMING CHEN, Nanyang Technological University, MINGLI JIA, Chinese Academy of Sciences, LI WEI, YUAN CHEN, M. B. CHAN-PARK, Nanyang Technological University, ANDONG XIA, Chinese Academy of Sciences — The optimal excitation wavelength for the energy transfer from aromatic polymers poly(9,9-dioctylfluorene-2,7-diyl) (PFO) to single-walled carbon nanotubes (SWNTs) is tunable in a wide wavelength range (from 388 to 480 nm) depending on the concentration of excess PFO polymers. The concentration governs the aggregation state and chain conformation of the polymers proximate to SWNT surfaces, which in turn alters the optical excitation wavelength. This study suggests an exciting and convenient method of adjusting the desired optical wavelengths for the energy conversion, useful for polymer-SWNT composites in optoelectronic applications.
4:54PM T24.00009 Exciton Dynamics in (6,5) carbon nanotubes, ANDY WALSH, JUDE SCHNECK, Boston University, ALEX GREEN, MARK HERSAM, Northwestern University, SIDNEY REDNER, LAWRENCE ZIEGLER, ANNA SWAN, Boston University — Single color (E22) pump-probe data on a solution of (6,5) nanotubes reveal that use of pulses shorter than the dephasing time scale precludes the formation of multiple excitons on a single nanotube. Subsequent relaxation dynamics of the single exciton exhibits stretched exponential behavior, and data from low to saturation fluence, and over 3 order of magnitude of time delay, is described by the same model. The stretched exponential model implies a distribution of decay rates is attributed to a distribution of length-dependent effective lifetimes due to end-quenching via diffusion. Results give values for the dipole moment, E22 dephasing time and E11 diffusion coefficient.

5:06PM T24.00010 Exciton Dynamics in Individual Single-walled Carbon Nanotubes, MARAT KHAFIZOV, SHUJING WANG, LISA J. CARLSON, TODD D. KRAUSS, Department of Chemistry, University of Rochester, Rochester, New York 14627, MING ZHANG, DuPont Central Research and Development, Experimental Station, Wilmington, Delaware 19880 — Optical excitation of single-walled carbon nanotubes (SWNTs) results in strongly bound excitons. The dynamics and energetic pathways available to the exciton as it relaxes back to the ground state have recently received significant attention. We have performed transient absorption (TA) experiments on DNA-wrapped (6,5) SWNTs in the extremely low-excitation fluence regime. Excitation was provided by a Ti-sapphire oscillator whose output was focused into a highly nonlinear photonic crystal fiber generating a coherent, femtosecond white-light source. We found the recovery of the photobleach signal for excitons in the 1st and 2nd excited states (E11 and E22) was governed by power-law dynamics. Interestingly, we also observed an induced absorption feature in the TA spectrum to the blue of the E11 exciton that showed the same recovery dynamics as the photobleach signal, suggesting that they share a common origin. We will discuss the physical origins of the observed features in the TA spectrum in the context of current models of exciton states of the SWNT.

Wednesday, March 18, 2009 2:30PM - 4:54PM

2:30PM T25.00001 Scanning Kelvin Probe Study of Electric Field Effect Tuning of Graphene, JESSE BEREZOVSKY, ROBERT WESTERVELT, Harvard University — Experiments on the transport properties of graphene over the last several years have revealed numerous unusual and fascinating results. These studies typically rely on lithographically patterned contacts and gates that can obscure effects arising due to spatially varying properties. Using a biased scanning probe tip, we can create a local gate or scattering potential and observe the resulting change in the transport properties of a graphene structure. Simulations show that this technique can image the fluctuating potential in a graphene nanoribbon, which shows promise for imaging the flow and behavior of electrons in graphene devices.

2:42PM T25.00002 STM Studies of Graphene Films Prepared by Sonication-Assisted Dispersion, ELENA STOLYAROVA, KWANG TAEG RIM, GEORGE FLYNN, Columbia University, COLUMBIA UNIVERSITY TEAM, COLUMBIA UNIVERSITY, COLUMBIA UNIVERSITY TEAM, POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — We present experimental work on the work function variation of mono and bi-layer graphene device measured by scanning Kelvin probe microscopy (SKPM). Using the electric field effect (EFE), the work function of graphene can be adjusted as the gate voltage tunes the Fermi level across the charge neutrality point. Mono and bi-layer graphene samples are deposited on a silicon oxide covered silicon substrate by a mechanical exfoliation method and electrical contacts are fabricated by electron beam lithography. The underlying silicon substrate is used as a back gate to tune the carrier concentration of the graphene. After subtracting off the large background signal originating from the electrostatic environment, we obtain the work function of graphene samples modulated by the gate voltage. The change of work function can be ascribed by the Fermi level shift due to the EFE induced carrier doping and well quantified by the electronic band structure of mono and bi-layer graphene.

3:06PM T25.00004 Low temperature scanning probe imaging of electron transport in graphene nanostructures, JESSE BEREZOVSKY, ROBERT WESTERVELT, Harvard University — Experiments on the transport properties of graphene over the last several years have revealed numerous unusual and fascinating results. These studies typically rely on lithographically patterned contacts and gates that can obscure effects arising due to spatially varying properties. Using a biased scanning probe tip, we can create a local gate or scattering potential and observe the resulting change in the transport properties of a graphene structure. Simulations show that this technique can image the fluctuating potential in a graphene sheet with a spatial resolution of tens of nanometers. By patterning the graphene into a nanowire or nanoconstriction, the local potential of the tip may be used to probe the dependence of the confinement-induced energy gap on the local atomic structure of the edges. These types of measurements provide a means for directly imaging the flow and behavior of electrons in graphene devices.

1:This work is supported by Global Research Laboratory and FENA

2:Work supported by Lucent, DE-FG02-99ER45742 and NSF-DMR-0456473

3:We acknowledge support from the DOE.
The flakes were characterized using a homebuilt, room temperature, ultrahigh-vacuum scanning tunneling microscope. We report on the apparent electronic in situ the Dry Contact Transfer (DCT) method [1] to deposit nanometer-sized, monolayer graphene flakes, using scanning tunneling microscopy.


Rutter, et al [3]. Room-temperature scanning tunneling spectroscopy (STS) measurements of the graphene monolayers and bilayers on the Si(111)-7x7 surface that the electronic structure of a graphene monolayer on the Si(111)-7x7 surface leads to the transparency of monolayers and bilayers, similar to the findings of clean Si(111)-7x7 surfaces. The DCT method deposits single, double, and thicker layers of atomically clean graphene. We observe varying degrees of transparency in the dI/dV measurement. This is in contrast to traditional magnetic oscillations which typically only probe the Fermi level. This work was supported in part by NSF, NRI-INDEX, and the W. M. Keck Foundation.

3:42PM T25.00007 Magnetic Oscillations in Scanning Tunneling Spectroscopy of Epitaxial Graphene on SiC . KEVIN D. KUBISTA, DAVID L. MILLER, GREGORY M. RUTTER, MING RUAN, WALT A. DE HEER, PHILLIP N. FIRST, Georgia Institute of Technology, JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology, NIST — Scanning tunneling microscopy (STM) and spectroscopy (STS) at a temperature of 4 K are used to study the electronic properties of epitaxial graphene on SiC in a magnetic field perpendicular to the graphene plane. While changing the magnetic field we observe Shubnikov de Haas-like magnetic oscillations in the tunneling conductance, dI/dV. The peak positions of these tunneling magnetic oscillations (TMO) vary periodically with inverse magnetic field, indicating they sample a constant cross-section of the graphene k-space. This new magnetic oscillation method can map extended parts of the electronic band structure of graphene as we vary the tunneling energy in the dI/dV measurement. We analyze our results in terms of graphene 2D electronic structure.

4:06PM T25.00009 Kondo Effect for Massless Dirac Fermions in Graphene1 , L. S. MATTOS, C. R. MOON, P. B. VAN STOCKUM, J. C. RANDEL, H. C. MANOHARAN, Stanford University, M. W. SPRINKLE, C. BERGER, W. A. DE HEER, Georgia Tech, K. SENGUPTA, SINP, A. V. BALATSKY, LANL — We experimentally probe the addition of the spin degree of freedom to the local physics of graphene. This real spin degree of freedom is expected to become intertwined in various coherent scattering processes involving pseudospin and chirality intrinsic to single monolayers of graphene. A Compendium of theoretical work on the interaction of localized spins with Dirac electrons predicts that low-temperature screening of localized magnetic moments by nodal quasiparticles gives rise to an unconventional Kondo effect, in which a critical exchange coupling can be controlled by charge carrier doping. We report the observation of this elusive Kondo ground state of Dirac particles, using scanning tunneling microscopy of adsorbed magnetic atoms on epitaxial graphene at low temperature. Tunneling spectroscopy and quasiparticle interference maps reveal chiral, linearly dispersing carriers by charge carrier doping. We report the observation of this elusive Kondo ground state of Dirac particles, using scanning tunneling microscopy of adsorbed magnetic atoms on epitaxial graphene at low temperature. Using Fourier-transform scanning tunneling spectroscopy and concomitant measurements in a high magnetic field, we deduce the origin of these features. We further probe atomic scale variations in the LDOS of graphene caused by impurities on the surface. We analyze our results in terms of graphene electronic structure.

1We acknowledge support from DOE

4:18PM T25.00010 Atomic-scale scanning tunneling microscopy and spectroscopy studies of nanometer-sized graphene on the Si(111)-7x7 surface . JUSTIN KOEPKE, JOSEPH LYDING, University of Illinois at Urbana-Champaign — We have used ultrahigh vacuum scanning tunneling microscopy to perform atomic-level studies of graphene on the Si(111)-7x7 surface. We used a dry contact transfer technique (DCT) developed by Albrecht and Lyding [1] to deposit mechanically exfoliated graphene in-situ [2] onto atomically clean Si(111)-7x7 surfaces. The DCT method deposits single, double, and thicker layers of atomically clean graphene. We observe varying degrees of transparency of the graphene monolayers and bilayers on the Si(111)-7x7 surface, where the substrate atomic structure is clearly seen through the graphene. We believe that the electronic structure of a graphene monolayer on the Si(111)-7x7 surface leads to the transparency of monolayers and bilayers, similar to the findings of Rutter, et al [3]. Room-temperature scanning tunneling spectroscopy (STS) measurements of the graphene monolayers and bilayers on the Si(111)-7x7 surface show predominantly metallic behavior. [1] P.M. Albrecht and J.W. Lyding, Appl. Phys. Lett. 83, 5029 (2003) [2] K.A. Ritter and J.W. Lyding, Nanotechnology 19, 015704 (2008) [3] G.M. Rutter, et al, Phys. Rev. B 76, 235416 (2007)

4:30PM T25.00011 Atomic-scale studies of nanometer-sized graphene on III-V semiconductors using scanning tunneling microscopy . KEVIN HE, JUSTIN KOEPKE, JOSEPH LYDING, University of Illinois - Urbana — We utilize the Dry Contact Transfer (DCT) method [1] to deposit nanometer-sized, monolayer graphene flakes, in situ, onto cleaved GaAs (110) and InAs (110) surfaces. The flakes were characterized using a homebuilt, room temperature, ultrahigh-vacuum scanning tunneling microscope. We report on the apparent electronic semi-transparent of the monolayer graphene flakes, such that the underlying III-V semiconductor lattice is revealed in our topographic images. This transparency is strongly dependent on the applied sample bias, similar to results seen on SiC (1000) for large sheets of graphene grown via thermal desorption [2].

I. Forbeaux et al. [1] have shown that the growth of graphene on Cu(001) leads to applications in future scalable graphene nano-electronics devices.

II. Chemical exfoliation of graphite in solvent of 1-pyrenecarboxilic acid in water. We confirm the presence of monolayer graphene sheets by Scanning transmission electron microscopy (STM) analysis. However, chemical approaches for high-yield production of graphene sheets is still absent. Here, we report that graphene dispersion produced by mechanical methods, exfoliation, epitaxial growth method and reduced graphene from two-dimensional crystallographic nature, which have resulted in intensive investigations of fundamental physics and promising applications. Up to now, several techniques have been used to produce small areas of graphene, such as mechanical methods, exfoliation, epitaxial growth method and reduced graphene from two-dimensional crystallographic nature, which have resulted in intensive investigations of fundamental physics and promising applications. The predicted supersaturation is highly nonlinear. Such behavior can be explained if carbon clusters must form as precursors to carbon attachment. As experiment and theory reveal, this could arise from strong bonding of monolayer monomers to the metal substrate.

III. We study the epitaxial growth of graphene on Ru(0001) measuring simultaneously the growth rate of individual graphene islands and the local, absolute concentration of vapor-deposited, mobile carbon adatoms. We have learned what controls the nucleation and growth rate of graphene, and what species transport carbon over the metal surface. We find that the growth rate is limited by C-atom attachment, not by C-atom diffusion, and that the absolute value of the supersaturation required for appreciable growth rates is comparable to that required to nucleate new islands. Thus, a step flow mechanism is unlikely to exist in monolayer graphene growth. The growth rate as a function of supersaturation is highly nonlinear. Such behavior can be explained if carbon clusters must form as precursors to carbon attachment. As experiment and theory reveal, this could arise from strong bonding of monolayer monomers to the metal substrate. We will discuss a model that explains and provides insight into the molecular processes by which graphene grows. This research is supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U. S. D. O. E. under Contract No. DE-AC04-94AL85000.

IV. Large scale graphene synthesized on metal and transferred to insulators: Material and Electronic Properties. YONG P. CHEN, H. CAO, D. PANDEY, I. CHILDRES, D. ZEMLYANOV, V. DRACHEV, R. REIFENBERGER, Purdue University, Q. YU, S. H. Y. LEE, University of Houston, J. LIAN, RPI, H. LI, University of Missouri — We report a systematic study of the material and electronic properties of large scale graphene films grown on metal and transferred to insulator substrates. Few-layer graphene films as large as several cm’s in size are grown by cooling-induced surface segregation on Ni under ambient pressure (Q. Yu et al., APL 93, 113103 (2008)). The Ni is subsequently etched by acid and graphene film transferred on thin SiO$_2$ on doped Si wafer. TEM and STM images show the expected graphitic lattice structure locally with atomic resolution. XPS and Raman spectroscopies further confirm the high quality of transferred graphene films. At larger scale, various SPM and optical imaging reveal non-uniform thickness and considerable height fluctuation, with the film consisting with domains (~1 μm in size) separated by elevated ridges. Using the doped Si as backgate, we observe moderate field effect in such transferred graphene films. Magnetotransport at variable temperatures show negative magnetoresistance at low magnetic field and characteristic features of weak localization in graphene, allowing us to extract information on carrier scattering in such large scale graphene.

V. Epitaxial Graphene on Co(0001) Probed by STM Measurements and First Principles Calculations. DEBORAH PREZZI, Columbia University (NY-USA) & S3-CNR-INFM (Modena - ITALY), DA-JIN EOM, KWANG T. RIM, HUI ZHOU, MICHAEL LEFENFELD, COLIN NUCKOLLS, Columbia University, MARK HYBERTSEN, Brookhaven National Laboratory, TONY HEINZ, GEORGE FLYN, Columbia University — Structural and electronic properties of finite-sized graphene patches on Co(0001) have been investigated through a combined experimental and theoretical characterization. The analysis of low-temperature scanning tunneling microscopy images establishes an atomically uniform epitaxial configuration of graphene on the Co surface in which a C atom is atop the interface Co atom, in agreement with total energy calculations based on a density-functional theory (DFT) approach. Scanning tunneling spectroscopy measurements show that the electronic properties of the interface are significantly different than both the clean Co surface and isolated graphene, suggesting a strong electronic coupling at the interface. DFT calculations provide a detailed analysis of the spectroscopic features in terms of spin and site contributions and reveal the coupling between graphene p and Co d states.

Wednesday, March 18, 2009 2:30PM - 5:30PM –
Session T26 DMP: Focus Session: Graphene XII: Synthesis and Growth 328

2:30PM T26.00001 Evidence for graphene growth by C cluster attachment. ELENA LOGINOVA, NORMAN C. BARTEL, PETER J. FEIBELMAN, KEVIN F. MCCARTY, Sandia National Laboratories — Until now the detailed mechanisms of graphene growth have not been experimentally determined, owing to limitations of the available experimental techniques. We study the epitaxial growth of graphene on Ru(0001) measuring simultaneously the growth rate of individual graphene islands and the local, absolute concentration of vapor-deposited, mobile carbon adatoms. We have learned what controls the nucleation and growth rate of graphene, and what species transport carbon over the metal surface. We find that the growth rate is limited by C-atom attachment, not by C-atom diffusion, and that the absolute value of the supersaturation required for appreciable growth rates is comparable to that required to nucleate new islands. Thus, a step flow mechanism is unlikely to exist in monolayer graphene growth. The growth rate as a function of supersaturation is highly nonlinear. Such behavior can be explained if carbon clusters must form as precursors to carbon attachment. As experiment and theory reveal, this could arise from strong bonding of monolayer monomers to the metal substrate. We will discuss a model that explains and provides insight into the molecular processes by which graphene grows. This research is supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U. S. D. O. E. under Contract No. DE-AC04-94AL85000.

2:42PM T26.00002 Large Scale Graphene Synthesized on Metal and Transferred to Insulators: Material and Electronic Properties. YONG P. CHEN, H. CAO, D. PANDEY, I. CHILDRES, D. ZEMLYANOV, V. DRACHEV, R. REIFENBERGER, Purdue University, Q. YU, S. H. Y. LEE, University of Houston, J. LIAN, RPI, H. LI, University of Missouri — We report a systematic study of the material and electronic properties of large scale graphene films grown on metal and transferred to insulator substrates. Few-layer graphene films as large as several cm’s in size are grown by cooling-induced surface segregation on Ni under ambient pressure (Q. Yu et al., APL 93, 113103 (2008)). The Ni is subsequently etched by acid and graphene film transferred on thin SiO$_2$ on doped Si wafer. TEM and STM images show the expected graphitic lattice structure locally with atomic resolution. XPS and Raman spectroscopies further confirm the high quality of transferred graphene films. At larger scale, various SPM and optical imaging reveal non-uniform thickness and considerable height fluctuation, with the film consisting with domains (~1 μm in size) separated by elevated ridges. Using the doped Si as backgate, we observe moderate field effect in such transferred graphene films. Magnetotransport at variable temperatures show negative magnetoresistance at low magnetic field and characteristic features of weak localization in graphene, allowing us to extract information on carrier scattering in such large scale graphene.

2:54PM T26.00003 Investigation of the early stages of graphene formation on 6H-SiC. J. R. SKUZA, Department of Physics, College of William and Mary, C. CLAVERO, K. YANG, Department of Applied Science, College of William and Mary, B. WINCHESKI, NASA Langley Research Center, R. A. LUKASZEWS, Departments of Applied Science and Physics, College of William and Mary — The predicted and/or observed unique properties of graphene have sparked tremendous research efforts to develop graphene-based ultra-high speed electronic and optical devices. The most promising technique to fabricate epitaxial graphene at the surface is via a high temperature sublimation of atomic layers of Si from monocrystalline SiC substrates [1,2]. However, this approach leads to rough surfaces and little work has been done to investigate graphene nucleation during the early stages of growth. We have used atomic force microscopy, scanning electron microscopy, and Raman spectroscopy to investigate the early stages of graphene nucleation and surface evolution when annealing semi-insulating and n-type doped 6H-SiC substrates under low vacuum (~ 10$^{-3}$ Torr) and ultra-high vacuum (10$^{-9}$ Torr) regimes. Scaling laws applied to the surface evolution in these two cases will be compared. [1] I. Forbeaux et al., Phys. Rev. B 58, 16396 (1998). [2] C. Berger et al., J. Phys. Chem. B 108, 19912 (2004).

3:06PM T26.00004 High-field production of graphene sheets by chemical exfoliation of graphite. XIAOHONG AN, SWASTIK KAR, MORRIS WASHINGTON, SAROJ NAYAK, Rensselaer Polytechnic Institute, DEPARTMENT OF PHYSICS, APPLIED PHYSICS AND ASTRONOMY TEAM — Graphene, a single atomic layer of graphite, has attracted vast interest recently owing to its perfect two-dimensional crystallographic nature, which have resulted in intensive investigations of fundamental physics and promising applications. Up to now, several techniques have been used to produce small areas of graphene, such as mechanical methods, exfoliation, epitaxial growth method and reduced graphene from graphitic oxide. However, chemical approaches for high-field production of graphene sheets is still absent. Here, we report that graphene dispersion produced by chemical exfoliation of graphite in solvent of 1-pyrenecarboxilic acid in water. We confirm the presence of monolayer graphene sheets by Scanning transmission electron microscopy and Raman spectroscopy. Large area of graphene sheets on SiO$_2$/Si substrate can be obtained by evaporating the graphene dispersion in oven and rinsing with methanol. We demonstrate the high-field production of graphene sheets by optical microscopy and scanning electron microscopy. Electrical and other applications of graphene developed this way are currently being investigated. This new graphene processing of chemical exfoliation of graphite could lead to applications in future scalable graphene nano-electronics devices.

3:18PM T26.00005 Scalable chemical vapor deposition of single- and few-layer graphene. LEWIS GOMEZ DE ARCO, YI ZHANG, AKSHAY KUMAR, CHONGWU ZHOU, University of Southern California — We report the implementation of a simple and scalable method to prepare single and few-layer graphene films by chemical vapour deposition. Micro Raman spectroscopy analysis of the synthesized films revealed the presence of single and few-layer graphene domains throughout the substrate. Synthesized graphene films were recovered on Si/SiO$_2$ substrates where back-gated FETs were fabricated. Four-probe measurements revealed sheet resistance of ~68 kΩ/sq for the recovered films. $I_{DS}$-$V_{DS}$ and transfer characteristics indicate a weak p-type behavior in the films and weak modulation of the drain current by the gate bias.
Temperature-dependence of Epitaxial Graphene Formation on SiC(0001)\textsuperscript{1}

LUXMI LUXMI, NISHHTHA SRIVASTAVA, PATRICK FISHER, RANDALL FEENSTRA, Carnegie Mellon University, JAKUB KEDZIERSKI, MIT Lincoln Laboratory, YUGANG SUN, Argonne National Laboratory, GONG GU, Sarnoff Corporation — The formation of epitaxial graphene on SiC(0001) (the Si-face) is studied using atomic force microscopy, Auger electron spectroscopy, low energy electron diffraction/microscopy, Raman spectroscopy, and electrical measurements. Starting from hydrogen-etched surfaces, graphene formation by vacuum annealing is observed to begin at about 1150 °C, with the overall step-terrace arrangement of the H-etched surface being preserved but with significant roughness (pit formation) on the terraces. At temperatures near 1350 °C, the surface morphology changes into relatively large flat terraces covered with several layers of graphene and containing a few large pits, with the terraces separated by step bunches. On the terraces the graphene thickness varies by typically ±1 monolayer. At higher temperatures the graphene film is observed to buckle and break up, presumably due to thermal mismatch with the SiC. Field-effect mobilities as high as 4200 cm\(^2\)/Vs for few-layer graphene films are found.

\textsuperscript{1}Supported by NSF, DARPA, and DOE (ANL). Opinions are those of the authors and not necessarily endorsed by the funding sources.

3:42PM T26.00007 Epitaxial Graphene Formation on SiC(0001)\textsuperscript{1}, NISHHTHA SRIVASTAVA, LUXMI LUXMI, PATRICK FISHER, RANDALL FEENSTRA, Carnegie Mellon University, JAKUB KEDZIERSKI, MIT Lincoln Laboratory, YUGANG SUN, Argonne National Laboratory, GONG GU, Sarnoff Corporation — The formation of epitaxial graphene on SiC(0001) (the C-face) is studied using atomic force microscopy, spatially resolved Auger electron spectroscopy, low energy electron diffraction, Raman spectroscopy, and electrical measurements. Starting from hydrogen-etched surfaces, graphene formation by vacuum annealing is observed over the temperature range 1200-1400 °C. Unlike the situation for the Si-face, it is found for the C-face that the initial graphene formation is three-dimensional. Micron-size islands with height of several nm are formed, with the graphene being thinner on these islands than between the islands. At higher formation temperatures the graphene layer becomes relatively flat, and has typical thickness of ∼10 monolayers. Electron diffraction indicates rotational disorder, with ±15 °-oriented spots observed in addition to the known ±2.2 °-spots. Field-effect mobilities as high as 4400 cm\(^2\)/Vs for multi-layer graphene films are found, with relatively good homogeneity over the wafer. \cite{Hass2008}.

\textsuperscript{2}Supported by NSF, DARPA, and DOE (ANL). Opinions are those of the authors and not necessarily endorsed by the funding sources.

3:54PM T26.00008 Band-gap tuning through progressive oxidative of graphene\textsuperscript{1}, TANESH BANSAL, ADITYA MOHITE, BRUCE ALPHENAAR, JACEK JASINSKI, MAHENDRA SUNKARA, University of Louisville, IAMRE, DEPT OF CHEM ENGG COLLABORATION — Graphene has a high electron mobility at room temperature, making it attractive for device applications. Because graphene is a zero-gap semiconductor, it is challenging to modulate its conductance using a field effect gate. Oxidation of graphene opens up a band gap, transforming oxidized graphene into an insulator. However, theory also suggests that there are a range of stable oxidation states corresponding to different oxygen coverage on the surface. Here, we demonstrate that it is possible to tune the band-gap of oxidized graphene by varying the surface oxygen concentration. Commercially obtained KISH graphite was converted to graphite oxide by treatment with a mixture of sulfuric acid and nitric acid. Oxidized graphene sheets were dispersed on quartz substrates following sonication and centrifugation of the graphite oxide. Using photocurrent spectroscopy the energy gap of individual oxidized graphene flakes were observed to increase from 0.62 eV to 0.69 eV with increasing oxidation time. Band-gap measurements were correlated with the surface oxygen concentration using XPS, UPS and FTIR.

\textsuperscript{3}Supported by NSF MRSEC DMR-0520020, JSTO DTRA, and ARO W911NF-06-1-0462.

4:06PM T26.00009 Electrical Characterization of Reduced Epitaxial Graphene Oxide\textsuperscript{1}, YIKE HU, XIAOSONG WU, MICHAEL SPRINKLE, NERASOA MADIOMANANA, MING RUAN, CLAIRE BERGER, WALTER DE HEER, Georgia Institute of Technology — We present results for on-chip oxidation of epitaxial graphene and sequential reduction of the insulating graphene oxide layers. In our previous work, we have used the Hummer’s method to oxidize epitaxial graphene and used electron beam exposure and heat treatment to reduce the epitaxial graphene oxide (EGO) band gap by changing the degree of oxidation. Here we further explore various oxidative and reduction methods on epitaxial graphene. EGO is characterized by atomic force microscopy, low-energy electron diffraction, ellipsometry, and Raman Spectroscopy. Mobility measurements of patterned structures are presented where epitaxial graphene layers pads are seamlessly connected to EGO ribbons.

\textsuperscript{3}This work was supported by the JSTO DTRA and the Army Research Office Grant # W911NF-06-1-0462 (ZL), and by the Nano/Bio Interface Center through the National Science Foundation DMR-0425780 (YL).

4:18PM T26.00010 Preparation of macroscopic graphene oxide membranes\textsuperscript{1}, ZHENTANG LUO, YE LU, LUKE SOMERS, A.T. CHARLIE JOHNSON, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA — Graphene oxide membranes up to 2000 square micrometers in size can be synthesized with ≥90 % yield in bulk quantities through a microwave assisted chemical method. Membranes are readily visualized on oxidized silicon substrate, which enables efficient fabrication of electronic devices and sensors. Field effect transistors made of the membrane show ambipolar behavior, and their conductivity is significantly higher than previously reported values.

\textsuperscript{3}Supported by NSF MRSEC DMR-0520020, JSTO DTRA, and ARO W911NF-06-1-0462.

4:30PM T26.00011 Optical and diamagnetic anisotropy of graphene oxide\textsuperscript{1}, A.L. EXARHOS, P.M. VORA, Z. LOU, A.T. JOHNSON, J.M. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania — We have recently shown that graphene oxide (GO) emits a broad photoluminescence (PL) band in both solid and aqueous preparations. The origin of this PL is not yet well understood, but for absorptive and emissive optical processes originating in the two dimensional GO plane, one expects an in-plane polarization. Studies of optical anisotropy can therefore help to clarify the origin of the PL. Here we use a method of optical nanomagnetometry (Torrens, et al., JACS 129, p. 252 (2007)) to extract these quantities, also determining the magnetic anisotropy. We find that when aqueous preparations of GO are placed in a magnetic field, diamagnetically induced alignment leads to marked linear polarization anisotropy of absorbance and photoluminescence. By taking six optical measurements at each magnetic field, we are able to extract the intrinsic polarization anisotropies of optical absorption and emission of GO flakes and to quantify the orbital diamagnetic anisotropy. We discuss how these quantities give insight into electronic delocalization in these systems.

\textsuperscript{3}Supported by NSF MRSEC DMR-0520020, JSTO DTRA, and ARO W911NF-06-1-0462.

4:42PM T26.00012 Graphite oxide as a nanoscale dielectric\textsuperscript{1}, BRIAN STANDELEY, ANTHONY MENDEZ, California Institute of Technology, EMMA SCHMIDGALL, Imperial College London, MARC BOCKRATH, California Institute of Technology — Graphite oxide’s ease of deposition and graphene-like properties when chemically reduced make it a promising electronic material. To complement this effort, we are studying graphite oxide as a potential dielectric for nanoscale devices. While unreduced graphite oxide is known to have a sheet resistance in the GΩ range, its out-of-plane conductivity has yet to be measured. We have fabricated ultrathin capacitors from graphite oxide sheets, and will present our efforts to measure its leakage current and breakdown electric field, thus providing an assessment of its potential as a gate insulator.
4:54PM T26.00013 Diffusion and Self-alignment of Atomic Oxygens on the Graphene Surfaces: First Principles Calculations, TAKAZUMI KAWAI, YOSHIYUKI MIYAMOTO, Nano Electronics Labs., NEC Corp. — Graphene is attracting much attention for the application of nano-devices due to its interesting electronic properties and its robustness. For the device applications, it is very important to know the behaviors of atmospheric molecules such as adsorption, diffusion, and desorption on the graphene surface because the reaction with such chemicals cause the significant change in the electronic properties at Fermi level and even break the sp² network. Here, the oxygen is one of the most important impurities that we want to know and control the behavior. In this paper, we performed density function calculations for the diffusion of atomic oxygens on a graphene sheet in a periodic boundary condition. The results for a single atomic oxygen in our calculations are consistent with the previous works with cluster models. However, the favorable adsorption site for the next oxygen atom and diffusion barriers are completely different from them. The atomic oxygens prefer to align along armchair direction but not zigzag one. We will further discuss the stability and diffusion of the next oxygen atom on the other side of the graphene.

5:06PM T26.00014 Large area graphene growth on 6H-SiC(0001), I.I. JOHANSSON, C. VIROJANADARA, M. SYVÄJÄRVI, R. YAKIMOVA, IFM, Linkoping University, A.A. ZAKHAROV, T. BALASUBRAMANIAN, MAX-lab, Lund University — Large area graphene growth on commercial Si-face on-axis 6H-SiC(0001) is demonstrated in this work. Samples were produced in a prototype of an inductively heated furnace. The growth was carried out in strongly isothermal conditions at a temperature of 2000 °C and at an ambient argon pressure of 1 atm. The quality and thickness of the graphene layers grown, using this ex situ method, were investigated using PES, ARPES), LEED as well as LEEM, PEEM micro-LEED and micro-PES at specifically defined small areas. Our results show that single layer graphene is formed over quite large areas on the sample but that two different domains can exist on some parts. A comparison with an in situ graphene sample, prepared by resistive heating to 1275 °C, was made. The results then obtained were similar to earlier findings [1-2] and showed that the size of the graphene flakes were very small compared to those obtained on the samples prepared with our ex situ method.

[1] T. Ohta, F. El Gabaly, A. Bostwick, J.L. McChesney, K.V. Emtsev, A.K. Schmid, Th. Seyller, K. Horn, E. Rotenberg, New. J. Phys. to earlier findings [1-2] and showed that the size of the graphene flakes were very small compared to those obtained on the samples prepared with our ex situ method.

5:18PM T26.00015 Epitaxial graphene: Structure, growth and molecular interactions, ANDREW WEE, WEI CHEN, SIEW WAI POON, HAN HUANG, SHI CHEN, DONGCHEN QI, ENG SOON TOK, KIAN PING LOH, National University of Singapore — The discovery of graphene has opened up a new paradigm in nanoelectronics that could offer better performance than conventional semiconductor devices. We used in situ scanning tunnelling microscopy (STM), synchrotron synchrotron radiation techniques and density functional theory (DFT) calculations to investigate the structure of the various reconstructions of 6H-SiC(0001) prior to its thermal decomposition to form epitaxial graphene (EG). Using Co-decoration technique coupled with STM, the evolution of EG was found to preferentially begin at SiC step edges and occurs with the loss of Si and breakdown of the C-rich (hexagonal SiC) template, which provides the C source for graphene growth. The C-rich phase that forms at the interface acts as a buffer layer for graphene from the underlying bulk SiC. We show that the transition from monolayer to trilayer EG adopts a bottom-up growth mechanism. With increasing annealing temperature, the fluorescence yield of Si K-edge NEXAFS indicates an increase in disorder of Si atoms in the SiC substrate beneath the surface due to out-diffusion of Si atoms to the surface forming increased Si vacancies. We also show that EG thermally grown on 6H-SiC(0001) can be p-type doped via a novel surface transfer doping scheme by modifying the surface with the electron acceptor, F4-TCNQ.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T27 FLAP: Focus Session: Pulsed Laser Deposition of Electronic and Photonic Thin Films and Nanostructures 329

2:30PM T27.00001 Plasma Energetic in Pulsed Laser Deposition and Pulsed Electron Deposition1, SOLOMON KOLAGANI, Neocera, LLC, Beltsville, Maryland, USA — Surface bombardment by energetic particles strongly affects thin film growth and allows surface processing under non-thermal equilibrium conditions. Deposition techniques enabling energy control can effectively manipulate the microstructure of a film and site for the next generation of complex structures that incorporate metals, complex dielectrics, ferroelectrics, semiconductors and glasses. In the case pulsed ablation techniques such as Pulsed Laser Deposition (PLD) and Pulsed Electron Deposition (PED), the initial energetic s of the material flux are typically in the range of 100s of eV, much higher than the optimal values (≤ 10 eV) required for high quality film growth. To overcome this problem and to facilitate particle energy transformation from the original as-ablated to the one optimal for film growth, one needs to carefully select the ablation conditions, conditions for material flux propagation through a process gas (or vacuum) and location of the growth surface (substrate) within this flux. In this talk, I will discuss the energetics of the propagating materials flux in the case of PLD and PED, and identify parameters that require critical control for realizing optimum thin film growth. As an example, growth optimization of epitaxial GaN films is provided. PED is complementary to PLD and exhibits an important ability to ablate materials that are transparent to laser wavelengths typically used in PLD. Some examples include wide band gap materials such as SiO2, Al2O3, MgO etc. Both PLD and PED features can be integrated within a single deposition module. PLD-PED systems enable in-situ deposition of a wide range of materials required for exploring the next generation of complex structures that incorporate metals, complex dielectrics, ferroelectrics, semiconductors and glasses.

In collaboration with Mikhail Strikovski, Neocera, LLC.

3:06PM T27.00002 Interface-controlled thin film growth of conjugated polymers via pulsed laser deposition1, R.K. GUPTA, K. GHOSH, Missouri State University, SUCHI GUHA, University of Missouri-Columbia — Matrix-assisted pulsed laser evaporation, a derivative of pulsed laser deposition (PLD), is an alternative method of depositing polymer and biomaterial films that allows homogenous film coverage of high molecular weight organic materials for a layer-by-layer growth without any laser induced damage. Polyfluorene (PF1-based conjugated polymers have attracted considerable attention in blue-emitting displays. Di-octyl substituted polyfluorene (PF8), its copolymers, and thiophene-based polymers were deposited as thin films using matrix-assisted PLD by employing a KrF excimer laser. The optical and structural properties of these films are compared with spincoated films via Raman spectroscopy, absorption and photoluminescence. The Raman spectra of both PLD and spincoated films are similar indicating that the polymer films deposited via PLD maintain their molecular structure. We further discuss the application of interface-controlled PLD grown films in metal-insulator-semiconductor diodes and field-effect transistors.

1 In collaboration with Mikhail Strikovski, Neocera, LLC.

2 This work was supported by NSF-ECCS #0823563.
3:18PM T27.00003 Bi$_{0.4}$Ca$_{0.6}$MnO$_3$ Epitaxial Thin Films on Silicon for Electronic and Photonic Applications 1. VERA SMOLYANOVA, GRACE YONG, BENJAMIN HOFMANN, RAJESWARI KOLAGANI, Towson University, YONG LIANG, Motorola Labs — Thin films of rare-earth manganese oxides (manganites) are usually grown on oxide substrates. It is more challenging to grow thin films of these materials on technologically versatile silicon. Upon illumination with visible light, the resistivity of Bi$_{0.4}$Ca$_{0.6}$MnO$_3$ epitaxial thin films fabricated via PLD on oxide substrates decreases significantly in a wide temperature range due to the destruction of charge ordering. This makes Bi$_{0.4}$Ca$_{0.6}$MnO$_3$ thin films attractive for potential photonic and opto-electronic device applications. Having in mind device applications, we have extended our studies to Bi$_{0.4}$Ca$_{0.6}$MnO$_3$ epitaxial thin films grown on Si (001) with different buffer layers. The advantages of different buffer layer schemes on Si (001) will be discussed. Influence of deposition and annealing conditions on film photoresponse will be reported. Photoinduced and current induced effects in films grown on oxide substrates and on buffered Si substrates will be compared.

1 This work is supported by the NSF grant DMR-0348939.

3:30PM T27.00004 Photoinduced effects in Bi$_{1-x}$Ca$_x$MnO$_3$ thin films with different oxygen content 1. GRACE YONG, RAJESWARI KOLAGANI, KHIM KARKI, BENJAMIN HOFMANN, VERA SMOLYANOVA, Towson University — Doped rare-earth manganese oxides (manganites) attract interest due to a variety of electronic, magnetic, and orbital states and their drastic response to application of modest external fields. A photoinduced insulator to conductor transition in thin films of Bi$_{1-x}$Ca$_x$MnO$_3$ associated with melting of the charge ordering [1] is especially interesting for potential photonic and opto-electronic device applications. From this point of view it is important to know what factors influence the photoinduced effects. We have found that oxygen content of Bi$_{1-x}$Ca$_x$MnO$_3$ thin films significantly modify conductive, structural and photoinduced properties. The role of growing and annealing conditions will be discussed. The change in magnitude and lifetime of photoinduced changes in films with different oxygen content will be reported. The possible origin of these changes will be discussed. [1] V. N. Smolyanova at al., Phys. Rev. B 76, 104423 (2007)

3:42PM T27.00005 Strain-modulated Self-Assembly of Nanostructures within Epitaxial Thin-films via Pulsed Laser Ablation 1. AMIT GOYAL, SUNG-HUN WEE, YANFEI GAO, CLAUDIA CANTONI, KARREN MORE, YURI ZUEV, JUNSOO SHIN, ORNL — Nanocomposites comprising three-dimensionally (3D) ordered arrays of nanodots of one type of complex ceramic material embedded in another complex ceramic material are expected to exhibit novel physical properties, tunable by adjusting the overall composition, concentration, feature size and spatial ordering of the nanodots. Applications of such nanocomposites in the areas of multiferrics, photovoltaics, solid state lighting, ultra-high density storage and high temperature (high-Tc) superconductivity are of interest. A joint experimental, theoretical and computational study on achieving ordering via 3D self-assembly of nanodots of complex ceramic materials, such as 3D self-assembly of insulating BaZrO$_3$ (BZO) nanodots within high-Tc superconducting YBCO films, has been performed. Vertically or horizontally ordered arrays (or simultaneous ordering in both directions) of BZO nanodots within superconducting films have been made possible via strain modulation between nanodots. Experimental results obtained for novel nanocomposites for other applications involving perovskite-spinel mixtures such as CoFe2O4-BaTiO3, CoFe2O4-BiFeO3, etc. will also be presented. Such materials with ‘controlled self-assembly’ of nanostructures should find application in many areas.

3:54PM T27.00006 Efficiency and Plume Dynamics for Mid-IR Laser Ablation of Cornea 1. AROSHAN JAYASINGHE, BORISLAV IVANOV, M. SHANE HUTSON, Dept of Physics & Astronomy, Vanderbilt University — This paper reports ablation experiments on porcine corneal tissue using the Vanderbilt Mark III Free Electron Laser (FEL) and a tabletop Raman-shifted Alexandrite laser. These experiments were designed to test previous models that suggested wavelength and intensity dependent ablation mechanisms. In one test, we compare ablation efficiency and plume dynamics for two FEL wavelengths (λ=2.77, 6.45 μm) chosen such that different components of the tissue matrix act as the primary chromophore (water or protein respectively), while keeping the total absorption constant. We find small differences in ablation efficiency (with slightly more efficient ablation at 2.77 μm); no difference in shockwave propagation; and slightly more particulate matter in the plume at 6.45 μm. In a second test, we find that the Raman-shifted Alexandrite laser has similar ablation efficiency to the FEL in the 6-7 μm range — despite a ∼500-fold higher intensity. Although these results do not conform the previous model predictions, the findings do suggest that the Raman-shifted laser can be a viable alternative to the FEL for surgical applications.

1 Supported by DoD MPEF program (FA9550-04-1-0045).

4:06PM T27.00007 Pulsed-Laser Deposition of ZnO Thin Films and Heterostructures for Device Applications 1. DAVID NORTON, University of Florida — ZnO is a wide bandgap semiconductor being explored for transparent electronics, UV light emitting diodes, spin-based devices and chemical sensors. In this talk, we will discuss recent progress and understanding for carrier doping and interface formation in epitaxial ZnO thin films grown by pulsed-laser deposition. One of the critical issues for device applications is the formation of low resistivity, high carrier density p-type ZnO material for minority carrier injection. The behavior of acceptor dopants within the ZnO and ZnMgO matrices will be described. Discussion will include stability of transport properties, stabilization of surfaces, and device characteristics.

4:24PM T27.00008 Role of the top electrodes and their interfaces on the resistive switching behavior of epitaxial NiO thin films, S.R. LEE, J.H. BAK, Y.D. PARK, K. CHAR, Seoul National University, Korea, D.C. KIM, S. SEO, X.S. LI, G.S. PARK, Samsung Advanced Institute of Technology, Korea, R. JUNG, Kwangwoon Univ., Korea — Initial I-V characteristics of resistive switching behavior have been investigated with epitaxial NiO thin films grown on (100) SrRuO$_3$ by using Al, Pt, and CaRuO$_3$ as the top electrodes. SRO/NiO/Al and SRO/NiO/Pt require an electroforming process for the initialization of the resistive switching, while SrRuO$_3$/NiO/CaRuO$_3$ is initially in a low-resistance state. The temperature dependence of the initial I-V characteristics indicates that insulating layers exist at the NiO/Al and NiO/Pt interface, presumably broken by the electroforming process. On the other hand, SRO/NiO/Al does not show the resistive memory switching behavior despite the electroforming behavior. The resistive switching endurance is also dependent on the top electrodes. Our results suggest that the oxygen defects and their bonding energy with the top electrode metal play a critical role on the resistive switching behavior.

4:45PM T27.00009 Effect of cation substitution on the resistive switching behavior in epitaxial NiO, H.M. KIM, S.R. LEE, J.H. BAK, M.L. JO, Y.D. PARK, K. CHAR, Seoul N. Univ. — The resistive switching behavior of NiO has been extensively investigated due to the nonvolatile ReRAM device applications. In contrast to unipolar resistive switching of NiO grown on Pt, bipolar resistive switching is observed in NiO grown on SrRuO$_3$ (SRO). The unipolar switching has been explained by the formation and rupture of filamentary conduction with the Joule heating, while the bipolar switching is still controversial. Our previous study with epitaxial (epi) NiO, prepared under various growth conditions and electrodes, suggested that the oxygen defects at the NiO/top electrode (TE) interface may be responsible for the bipolar switching and TE may compensate the oxygen defects. In order to understand the role of the defect states at the interface on the resistive switching, 1-mm-thick epi-AI$_2$O$_3$ interlayer has been deposited on and under epi-NiO. The I-V characteristics have been investigated with an epi-CaRuO$_3$ (CRO) as TE, resulting in a clean interface with NiO. SRO/NiO/CRO shows poorer switching endurance in the less than 25% of measured cells. However, SRO/AI$_2$O$_3$/NiO/CRO exhibits bipolar switching in the most of measured cells with better endurance. This may imply the different oxygen defect states of each interface of NiO. As an effort to investigate the defect states in bulk and their effect on the unipolar switching, the I-V characteristics of Al substitution in epi-NiO will be presented.
The technique depends on the intensities of the laser pulses used, and propose a few candidate molecules for experimental tests of this concept. In this presentation, we will show results of computer simulations of this technique. We will show that even if the reaction rate constants are small, ground state. The result is that the molecules at the center of the pulses (in a region of size \( \lambda = 1064 \text{ nm}, 10 \text{ Hz repetition rate} \)) was used to ablate a Ge target. In-situ RHEED and STM and ex-situ AFM were used to study the morphology of the grown QD. The dependence of the QD morphology on substrate temperature and ablation and excitation laser energy density was studied. Electronic excitation is shown to affect the surface morphology. Laser irradiation of the Si substrate is shown to decrease the roughness of films grown at a substrate temperature of \( \sim 450 \text{ } ^\circ \text{C} \). Electronic excitation also affected surface coverage ratio and cluster density and decreased the temperature required to form 3-dimensional quantum dots. Possible mechanisms involved will be discussed.

Computer simulations of photochemistry controlled with subwavelength resolution\(^1\), TRIET NGUYEN, ALEX SMALL, California State Polytechnic University, Pomona — A technique called Stimulated Emission Depletion (STED) has recently been developed to beat the diffraction limit in imaging. We propose to adapt this technique to control chemical reactions with nanoscale resolution. We simulated a process in which a series of laser pulses is applied at each site on a surface. The first pulse excites the molecules and the second pulse (with a TEM10 “doughnut” profile) then causes the excited molecules away from the node at the center to undergo stimulated emission and return to the ground state. The result is that the molecules at the center of the pulses (in a region of size \(<<\lambda\)) remain in the excited state and can undergo chemical reactions. In this presentation, we will show results of computer simulations of this technique. We will show that even if the reaction rate constants are small, the application of several sequential pulses leads to a fractionation effect that compensates for low reaction rates. We will also show how the resolution of this technique depends on the intensities of the laser pulses used, and propose a few candidate molecules for experimental tests of this concept.

\(^1\)This work was funded by the Kellogg Honors College.

**Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T28 FIAP DMP: Focus Session: Thermoelectric Materials: Nanostructures**

**2:30PM T28.00001 SiGe Nanocomposites Thermoelectrics: The Knowns and the Unknowns**

GANG CHEN, Massachusetts Institute of Technology — Silicon-germanium has been used in spacecraft for a long time to convert heat from radio isotope heat sources into electricity for deep space missions. In this talk, we will discuss the current status of our understanding of thermoelectric transport in nanocomposites. Careful examination of the spectral details of the electron and phonon transport reveals a significant deficiency in our current understanding, even for bulk materials. Different interfacial transport processes further complicate the picture. In this talk, we will discuss the current status of our understanding of thermoelectric transport in nanocomposites. In collaboration with A. Minnich, H. Lee, B. Muralidharan, and M.S. Dresselhaus, Massachusetts Institute of Technology, Cambridge, MA 02139; and X. W. Wang, G. Joshi, G. H. Zhu, Y. C. Lan, D. Z. Wang, and Z.F. Ren, Boston College, Chestnut Hills, MA 02467.

\(^2\)This work is supported by NSF Grant No. 0833150, DOE Grant No. DE-FG02-08ER46516, and Toyota.

**3:06PM T28.00002 Thermoelectric Power of high concentration embedded Nano-particle Samples**

MONA ZEBARJADI, KEIVAN ESFAJANI, ALI SHAKOURI, ZHIXI BIAN, University of California, Santa Cruz; JE-HYEOUNG BAHK, GEHONG ZENG, JOHN BOWERS, HONG LU, JOSHUA ZIDE, ART GOSSARD, University of California, Santa Barbara, UNIVERSITY OF CALIFORNIA, SANA CRUZ TEAM, UNIVERSITY OF CALIFORNIA, SANTA BARBARA TEAM — High concentrations of embedded nano-particles inside thermoelectric elements are desirable because they can increase the thermal conductivity. But they also affect the power-factor. Therefore they can enhance or suppress the figure of merit. We model the effect of such high concentrations on the power-factor using the coherent potential approximation. We optimize the power-factor versus nano-particle size, distribution and concentration. The analysis would help in designing nano-particle embedded matrices with high-performances. We characterize InGaAlAs samples with 3-10% volume concentration of ErAs nanoparticles and explain their properties such as the mobility and the Seebeck coefficient theoretically.

**3:18PM T28.00003 Transient Electrical and Thermal Characterization of InGaAlAs Thin Films with embedded ErAs Nanoparticles**

TELA FAVALORO, University of California, Santa Cruz School of Electrical Engineering, RAJEEV SINGH, JAMES CHRISTOFFERSON, YOUNES EZZAHRI, ZHIXI BIAN, ALI SHAKOURI, GEHONG ZENG, JE-HYEUNG BAHK, JOHN BOWERS, HONG LU, ARTHUR GOSSARD — We developed a system for accurate high-temperature characterization of thermoelectric materials and devices. This system can be used for electrical measurements of thermoelectric properties and contains an integrated optical thermoreflectance imaging system integrated into the thermostat for analysis of sample surface temperature profile resulting from the Peltier effect, Joule heating or external thermal excitation within the sample. Transient electrical and thermal measurements are useful to extract material diffusivity of each layer. We have performed high temperature transient analyses and thermal imaging of thin film devices optimized for direct figure of merit detection in the cross-plane direction. These devices consist of 25 micron thick samples of InGaAlAs films with embedded ErAs nanoparticles. Using the transient Harman technique, we determine the cross-plane figure of merit of each device. Heat sources are used to model the effect of such high concentrations on the power-factor using the coherent potential approximation. We optimize the power-factor versus nano-particle size, distribution and concentration. The analysis would help in designing nano-particle embedded matrices with high-performances. We characterize InGaAlAs samples with 3-10% volume concentration of ErAs nanoparticles and explain their properties such as the mobility and the Seebeck coefficient theoretically.

**3:30PM T28.00004 Characterization and modeling of the randomly distributed ErAs nanoparticles in InGaAlAs semiconductors for thermoelectric power generation**

JE-HYEUNG BAHK, UCSC, MONA ZEBARJADI, ZHIXI BIAN, UCSC, GEHONG ZENG, ASHOK RAMU, HONG LU, UCSC, ALI SHAKOURI, UCSC, ART GOSSARD, JOHN BOWERS, UCSC — We investigate temperature-dependent thermoelectric properties of the InGaAlAs semiconductors containing epitaxially embedded ErAs nanoparticles grown by Molecular Beam Epitaxy. Temperature-dependent Hall measurements and Seebeck coefficient measurements were performed for the materials with various Er concentrations and semiconductor compositions, and the results were analyzed using a theoretical modeling based on the ErAs nanoparticle’s carrier scattering behaviors. In the analysis, the nanoparticles are modeled as charged spheres with Schottky barrier height at the interface with semiconductor, and the potential profile around a particle is used as perturbation for electron scattering. The particle scattering rate is calculated using both Born approximation and the partial wave method, respectively, and the two methods are compared to check the validity of Born approximation in various conditions. The theoretical calculation of mobility and Seebeck coefficient based on the modeling of particle scattering and other scattering mechanisms fits the measurement results, and we find that further enhancement of thermoelectric power factor is possible by optimizing the particle scattering in the materials.
3:42PM T28.00005 Thermal and Thermoelectric Transport in Thin Films and Nanostructures

BO L. ZINK, R. SULTAN, A. D. AVERY, University of Denver — Interest in increasing efficiency of energy generation continues to spur the development of new thermoelectric materials. Though bulk materials hold the most promise for large-scale energy generation, many groups continue to explore increasing the thermoelectric figure-of-merit by taking advantage of techniques for creating nanostructured materials such as multilayered thin films and nanowires. These systems could prove to have high figures-of-merit and be important for integrating energy harvesting and/or cooling with micro- or nanoscale devices “on chip.” Though many promising systems have been identified, measuring their fundamental thermal transport often remains a major challenge. In this talk, we briefly describe our recent advances in measuring in-plane thermal transport, thermopower and electrical conductivity on thin-films or nanolithographically patterned systems. Our technique allows great flexibility for studying the thermoelectric properties of a wide range of materials, from amorphous semiconductors to semi-metallic nanowires.

We thank ACS-PRF, NERC, and the University of Denver for supporting this work


ROBERT WORTMAN, JEREMY SCHROEDER, POLINA BURMISTROVA, Birck Nanotechnology Center, Purdue University, MONA ŽEBARJADI, ZHIXI BIAN, ALI SHAKOUROUI, Department of Electrical Engineering, UC Santa Cruz, TIMOTHY SANDS, Birck Nanotechnology Center, Purdue University — A new class of thermoelectric materials based off of superlattices have been proposed that show a potential for enhanced thermoelectric performance. The increase of thermoelectric figure-of-merit ZT of these materials is due to both the energy filtering effect of the Schottky barriers as well as the reduced thermal conductivity that results from increased interface density. Our work has centered on the metal-semiconductor materials system of HfN-SnC. These are both high temperature materials (T_m > 2500°C). They have the same rocksalt crystal structure and similar lattice constants, allowing epitaxial growth. We have grown superlattices of these materials via DC magnetron sputtering. Results from x-ray diffraction, and electrical and thermal tests will be presented. Their potential as thermoelectric energy conversion materials will be discussed. I. G. D. Mahan et al, Phys. Rev. Lett., 80, 4016 (1998) 2 D. Vasas et al, Phys. Rev. Lett. 92, 106103 (2004)

4:06PM T28.00007 ABSTRACT WITHDRAWN

4:18PM T28.00008 Thermoelectric properties of nanoporous Ge

JOO-HYOUNG LEE, JEFFREY GROSSMAN, University of California-Berkeley — Recently, silicon nanowires were shown to have a thermoelectric (TE) figure of merit (ZT) two orders of magnitude larger than that of bulk Si. In addition, recent theoretical work predicted that Si with periodically arranged nanometer-sized pores (nanoporous Si) could result in a similar increase in ZT. These results open an exciting new pathway towards efficient thermoelectrics based on standard semiconductor materials. In the present work, we experimentally extend our earlier calculations on silicon to explore the TE properties of nanoporous Ge. Specifically, we calculate the thermal and electrical conductivities, Seebeck coefficient and figure of merit of nanoporous Ge for a range of configurations using a combined ab initio electronic structure calculation and Boltzmann transport approach. The results show a substantial increase in ZT compared with that of bulk Ge, as in the Si nanostructures. A detailed comparison between the TE properties of nanoporous Ge and Si will be presented.

1 A. I. Hochbaum et al., Nature 451, 163 (2009); A. I. Boukai et al., ibid., 451, 168 (2009)

4:30PM T28.00009 Solution processable routes to nanostructured thermoelectric materials

JOSEPH FESER, Department of Mechanical Engineering, University of California - Berkeley, ROBERT WANG, The Molecular Foundry, Lawrence Berkeley National Laboratory, LAWRENCE MAJUMDAR, Department of Mechanical Engineering, University of California - Berkeley, JEFFREY URBAN, The Molecular Foundry, Lawrence Berkeley National Laboratory — The previous decade of research has shown that nanostructured thermoelectric materials can have superior performance compared to their bulk counterparts. Often, the synthesis of nanostructured materials is performed by layer-by-layer methods, which hinders their ability to be produced as thick films. Here we show a scheme by which nanocrystals embedded in a thermoelectric matrix may be produced using solution processing. Using hydrazine chemistry, we prepare soluble precursors for Bi2O3 (X=S,Se,Te). Solutions containing those precursors are spun and drop-cast onto substrates, and their electrical and thermal properties are characterized. We show ongoing research to embed colloidal nanocrystals into a matrix made from the soluble precursors.

4:42PM T28.00010 Self-supporting (Bi0.11Sb0.29)(Te0.25Se0.41) nanowire arrays for thermoelectric microdevices

HATEM EL-MATBOULY, TIMOTHY SANDS, KALAPI BISWAS, Purdue University — Nanostructuring of thermoelectric material can lead to improved performance through suppression of the lattice contribution to thermal conductivity and enhancement of the power factor by quantum confinement or thermionic energy filtering. To take advantage of these effects in a Peltier microcooler or Seebeck generator, it is necessary to prepare nanostructure materials with leg lengths ranging from tens of microns to millimeters. We have developed a process for fabrication of thick, self-supporting (Bi0.11Sb0.29)(Te0.25Se0.41) nanowire arrays using a novel branched porous anodic alumina template that can be removed completely by selective etching following electrodeposition of the thermoelectric material, resulting in 100-micron-thick nanostructured thermoelectric material without the parasitic thermal shunt that is associated with the template. The electrodeposition process allows composition modulation and grading, effects that are difficult to achieve by bulk synthesis. Bandgaps of the electrodeposited material range from 0.13 eV for Bi2Te3 to an optical gap of 0.52 eV measured for a (Bi,Sb)(Te,Se) alloy, suggesting an operating temperature range from below room temperature to ~300°C.

4:54PM T28.00011 Thermoelectric Properties of Nanostructured n-type Yb3Co2Sb2Bulk

JIAN YANG, HUI WANG, YUCHENG LAN, XIAO YAN, BO YU, XIAOWEI WANG, GAOHUA ZHU, DEZHI WANG, ZHIFENG REN, Physics Department, Boston College, Chestnut Hill, MA 02467, QING HAO, GANG CHEN, Department of Mechanical Engineering, MIT, CAMBRIDGE, MA 02139, QIN-YU HE, South China Normal University, Guangzhou, CHINA MAIDRED S. DRESSELHAUS, Dept. of Electrical Engineering and Computer Science, Department of Physics, MIT, CAMBRIDGE, MA02139 — Nanostructured single phase of Yb3Co2Sb2 with a nominal composition of Yb3Co2Sb2 (X = 0.3, 0.35, 0.4, and 0.5) have been synthesized by ball milling and direct current induced hot press. Thermoelectric properties including electrical conductivity, Seebeck coefficient, and thermal conductivity from room temperature to 550°C were measured and discussed. It was found that Yb0.35Co2Sb2 has the optimal dimensionless figure of merit of 1.2 at 550°C.

5:06PM T28.00012 Thermoelectricity in Arrays of Thiolate Coated Au Nanoparticles

E. COVINGTON, F. BOHRER, E. T. ZELLERS, C. KURDACK, University of Michigan — We have developed a new technique to measure the thermopower of highly resistive films of thiolate coated Au nanoparticles. Using e-beam lithography, we fabricate two long parallel gold wires, spaced by 500 nm, on an insulating substrate and subsequently coat with a thin film of nanoparticles. The wires are used as electrodes for electronic conduction and heaters for thermopower measurements. We characterize the Joule heating in the wires using noise thermometry. To characterize the thermopower of the film, we excite one wire by an ac current with frequency . Due to Joule heating, we establish a temperature difference between the two wires modulated with frequency . We extract the thermopower by measuring the voltage signal between the wires using lock-in techniques. We used this method on Au nanoparticles with 1-octanethiol (C8) ligands where the thermopower was less than 10 µV/K at room temperature. From the sign of the thermopower, we determined transport was mainly due to tunneling of electrons through the lowest unoccupied molecular orbital of the C8 molecule.
5:18PM T28.00013 Molding Phonon Flow with Symmetry: Rational Design of Hypersonic Phononic Crystals

CHEONG YANG KOH, EDWIN L. THOMAS, Dept of Materials Science & Engineering, Massachusetts Institute of Technology — Phononic crystals structured at appropriate length scales allow control over the flow of phonons, leading to new possibilities in applications such as heat-management, sound isolation and even energy transfer and conversion. Symmetry provides a unified framework for the interpretation 1D to 3D phononic band structures, allowing utilization of a common set of principles for designing band structures of phononic crystals as well as actual purposeful defects such as waveguide location and boundary termination in finite devices. In this work, we explore the band structure properties of phononic crystals with non-symmorphic space groups, as well as those having quasi-crystalline approximants. We demonstrate gap opening abilities from both anti-crossing and Bragg scattering, as well as unique features like “sticking” bands. Symmetry concepts are also powerful means to tune the density of states of the structures. Importantly, we fabricate various theoretical designs and measure their experimental dispersion diagrams for comparison with theoretical calculation. This affords an elegant approach toward a design blueprint for fabricating phononic structures for applications such as opto-acoustic coupling.

Wednesday, March 18, 2009 2:30PM - 4:42PM —
Session T29 FEd: Focus Session: NSF’s Research Experience for Undergraduates (REU) Program: Overview and Perspectives 333

2:30PM T29.00001 Physics NSF-REU Site Director Workshop: What Did We Learn and What Questions Remain?1, MARIO AFFATIGATO, Coe College — The Research Experience for Undergraduates program, traditionally funded by the National Science Foundation and by other agencies (including the Department of Defense), has been a great success. Every year, hundreds of students have the chance to participate in research activities at Universities and research entities other than their own. These extended experiences have helped the students develop confidence in their abilities as practicing physicists, train on state of the art instrumentation, work on communication skills through presentations, and frequently reach a publication milestone. The REU program’s impact is manifold and complementary to the strong work done at the home institutions by faculty advisors and instructors. In this presentation we will discuss the current state of the program as determined by the recent (and first) meeting of the Physics REU site directors. In particular we will focus on the strengths of the program, shared good practices, data gathering, and some changes the new Steering Committee might implement. The intended audience should be current REU directors and faculty research supervisors; students who might be interested in the program; faculty at institutions who might be thinking of applying to become a site; and anyone attentive to undergraduate research in general.

3:06PM T29.00002 Past participant’s perspective on the Research Experience for Undergraduates program, DEREK PADILLA, San Diego State University — The Research Experience for Undergraduates (REU) programs funded by the National Science Foundation provide an outstanding opportunity for many students to participate in high-quality research at a facility other than their own institution. As a participant in the summer of 2006 I will attest to the success of a great REU program. This discussion will focus on my work and experience while in the program as well as the continuing relationship with my advisors and the host department as a whole. In collaborating with all levels of REU personnel we will improve the function of an already outstanding opportunity for undergraduate students for the coming years.

3:18PM T29.00003 Recuiting minority students into your REU program, DAVID ERNST, Vanderbilt University — It is important for the field of physics that we draw our talent from the broadest pool. However, African Americans, Hispanic Americans, and Native Americans are substantially underrepresented in physics. Since summer research experiences are a useful tool to assist students in gaining entrance into graduate school, it is particularly important that underrepresented minority students are fully able to participate. The NSF REU program at Vanderbilt University is historically comprised of one half minority students. How this comes about and how we pro-actively recruit minority students will be described.

3:30PM T29.00004 International Summer Research Program in Gravitational-Wave Physics operated by the University of Florida for the LIGO VIRGO Science Collaboration1, GUIDO MUELLER, BERNARD WHITING, University of Florida — The NSF-funded Laser Interferometer Gravitational-Wave Observatory (LIGO), 20+ US universities and colleges, and their international partners in Europe, Australia, and Japan are operating a network of six large scale interferometers to detect gravitational waves from neutron star or small black hole mergers, supernovae, and other galactic or cosmological sources. The data analysis as well as R&D activities for future gravitational-wave detectors are organized within the LIGO VIRGO Scientific Collaboration. This international frame provides the backdrop of our international summer research program. Our international partners offer currently up to 30 different research projects at 15 different institutions in 6 different countries on 3 different continents for US undergraduate students. Our primary target group are students from small US colleges who are active members of the LIGO Science Collaboration. In addition to the standard goal of exposing the students to cutting edge research, the students will also be exposed to a different culture (and usually language), and their research experience will help our small college groups to build-up or solidify their own research connection with our international partners. See http://www.phys.ufl.edu/reu for more details.

3:42PM T29.00005 REU in Physics at Kansas State University — an Evolving Program1, KRISTAN CORWIN, BRUCE GLYMOUR, AMY LARA, LARRY WEAVER, DEAN ZOLLMAN, Kansas State University — The REU site in the Physics Department at Kansas State University, funded by NSF for 13 years between 1992 and 2007, originally focused on atomic collision physics. Now the theme has broadened to include laser-matter interactions on atomic and nanoscales, and an ethics component is incorporated. Students study how atoms and molecules interact with ultra-fast optical and x-ray pulses, reveal the structure of nanoparticle crystallization and gel formation with scattered laser light, and develop computer codes for atomic interactions in Bose-Einstein condensates and nanoparticle self-assembly from lattices to gels; some have traveled to Japan for neutrino experiments. The students we select come primarily from smaller colleges and universities in the Midwest where research opportunities are limited. Prof. Weaver, who has served as PI since 1992, facilitates their transition from a teaching to research environment through lectures and individual interactions. Our program is in a period of transition. While Prof. Weaver continues to be the “impedance match” between students and mentors, other leadership roles are gradually being assumed by a team of faculty members who strive to preserve the intimacy and excellence of the program.

1Funded by the National Science Foundation Award No. 0552878.

1National Science Foundation, DoD, and other agencies are gratefully acknowledged for funding the REU program.
We acknowledge support from the NSF under Grant No. DMR-0646842.

Wednesday, March 18, 2009 2:30PM - 5:30PM –
Session T30 DMP GMAG: Focus Session: Excitations in Multiferroics 334

2:30PM T30.00001 Electromagnon spectra in multiferroic manganites $R\text{MnO}_3$, NOBUO FURUKAWA, Dept. of Physics, Aoyama Gakuin Univ., and ERATO-Multiferroics, JST — The magnetoelectric (ME) effect, in which electric polarization (magnetization) are controlled by magnetic (electric) field, have recently attracted intensive attention. One of the materials which exhibits large ME effects is the manganites $R\text{MnO}_3$. In this presentation I focus on electromagnon excitations (in a wide sense). In those manganites, cycloidal spin structures create ferroelectricity through spin-orbit couplings. Originally, electromagnon is defined as a collective excitation of spins in such a way that rotation of the cycloidal plane is driven by the electrical field of light coupled to the ferroelectric moment. Spectra for electrically excited magnons are indeed reported in TbMnO$_3$, GdMnO$_3$, (Eu,Y)MnO$_3$, and DyMnO$_3$. However, the selection rule observed in these compounds ($E^\parallel a$, irrespective of the cycloidal planes) is inconsistent with the theoretical prediction. Alternatively, couplings between electric field and spins through spin-dependent local polarizations have been proposed. I show both one- and two-magnon excitation spectra, and clarify consistencies and discrepancies of the model with experimental data. Roles of phonons and orbital orders in these compounds are also discussed.


3:06PM T30.00002 Selection rules for electromagnons in anharmonic cycloidal multiferroics$^1$, MARKKU STENBERG, ROGERIO DE SOUSA, University of Victoria — The coexistence of magnetic and ferroelectric phases in multiferroic materials gives rise to hybrid excitations with mixed magnetic and electric character. These excitations, so-called electromagnons, have been observed in several oxide materials, but their origin and optical selection rules are central questions that are not yet understood. We present a theory of electromagnon excitation in magnets with anharmonic cycloidal ground state. In contrast to previous theories, we show that multiple electromagnons are excited by light polarized along the cycloidal plane as well as perpendicular to it. Our results allow the distinction between different magnetoelastic couplings and have important implications for the interpretation of optical experiments in rare earth manganites as well as other materials with anharmonic spiral magnetic order.

$^1$We acknowledge support from NSERC and the University of Victoria - Faculty of Science

3:18PM T30.00003 Low-magnetic field control of electromagnon, N. KIDA, ERATO Multiferroics Project, S. ISHIWATA, Y. TAGUCHI, CMRG-RIKEN, R. SHIMANO, ERATO and Univ. Tokyo, T. ARIMA, Tohoku Univ., Y. TOKURA, ERATO, Univ. Tokyo, and CMRG-RIKEN — Since the 1960s, there has been intense debate concerning the presence of the spin excitation driven by the electric field of light $E^\parallel$ in ferromagnetic magnets. This is recently revived by the observation of the absorption peak structure around 3 meV in a ferroelectric magnet TbMnO$_3$ [1]. As an origin of this excitation, the hybridized spin excitation with electric polarization (now called electromagnon) was considered [2]. However, this issue remains controversial by our THz spectroscopic studies on a family of $R\text{MnO}_3$ [3] ($R = \text{Tb}, \text{Dy}$, and Gd), in a variety of spin phases tuned by temperature and magnetic field. Here we report an optical investigation of the low-energy ($\sim 10$ meV) spin dynamics for other ferromagnetic magnets, hexaferrite, by using THz time-domain spectroscopy. We find the signature of the genuine electromagnon at THz frequencies. As a manifestation of the strong magnetoelastic coupling inherent to the electromagnon, we demonstrate the low-magnetic field ($\sim 100$ Oe) control of the optical constants at THz frequencies. [1] A. Pimenov et al., Nat. Phys. 2, 97 (2006). [2] D. Senff et al., PRL 98, 137206 (2007). [3] N. Kida et al., PRB 78, 104414 (2008); Y. Takahashi et al., PRL 101, 187201 (2008); N. Kida et al., J. Phys. Soc. Jpn. Dec. issue (2008).
3:30PM T30.00004 Theory of novel one-magnon excitation induced by electric fields in cycloidal spin magnets. SHIN MIYAHARA, Japan Science and Technology Agency, NOBUO FURUKAWA, Aoyama Gakuin University — We propose a new mechanism to induce a novel one-magnon excitation by electric-field component of light in cycloidal spin states. We calculated optical spectra in the cycloidal spin structures as observed in multiferroic perovskite manganites. We showed that the novel excitation is driven by electric-field component of light is observed. When symmetric pairs of spins dependent electric polarizations are introduced, we have light absorptions at terahertz frequencies with one- and two-magnon excitations driven by electric-field components. Our results show that some parts of optical absorption peaks observed experimentally at terahertz frequencies are one-magnon excitation absorptions.

3:42PM T30.00005 Origin of electromagnons in multiferroic manganites. ROLANDO VALDES AGUILAR, Department of Physics, University of Maryland — The interest in multiferroic materials has increased in the last few years due to the fundamental physics of strong interaction between ferroelectric and magnetic orders, as well as for the promise of novel applications in future electronics. From powerful symmetry arguments and with modeling of the microscopic coupling mechanism, these efforts have led to the discovery of a vast set of multiferroic compounds. An important recent step in this regard was the discovery of a new kind of magnetic excitation that couples strongly to light by acquiring electric dipole activity from the infrared active phonons, called electromagnon, which is a hybrid excitation of magnon and phonon character. These discoveries have highlighted the importance of the dynamical aspects of the magnetoelectric coupling. Even though a wide consensus has been reached regarding the origin of the static magnetoelectric dynamic effect of electromagnons was not clear. In this talk a combination of theory and experiment is presented that clarifies the origin of the electromagnon excitations in RMnO3. This model is based on symmetric exchange striction and takes into account the lattice and magnetic symmetry of this family of perovskite manganites. It reproduces the fact that the observed selection rule for electromagnons in RMnO3 is independent of the spin plane. This result is due to the effective modulation of the exchange interaction between Mn spins induced by the electric field of light. The proposed mechanism is also related to the origin of static polarization in the E-phase of this RMnO3 multiferroic family. The model and experiments carried out so far demonstrate that the symmetric exchange interaction is responsible for all the observed dynamical magnetoelectric effects, and opens a new avenue for study of these multiferroic compounds.

4:18PM T30.00006 Infrared-active excitations related to the $R^{3+}$ ligand-field splitting in $RMn_2O_5$ ($R$=Ho, Dy, Tb). A. A. SIRENKO, S. M. O’MALLEY, T. D. KANG, K. H. KAHN, Department of Physics, NJIT, Newark, NJ, C. L. CARR, NSLS, Brookhaven National Laboratory, Upton, NY, L. MIHALY, Department of Physics and Astronomy, Stony Brook University, NY, S. PARK, S.-W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, NJ — Optical transitions between ligand-field split states of $R^{3+}$ ions in $RMn_2O_5$ multiferroic single crystals have been studied at the phase transitions in the external magnetic field up to 13 T and uniaxial pressure up to 5 kbar. Spectra of the ligand field excitations change significantly in external magnetic field and correlate with the reversal of electric polarization induced by magnetic field. The oscillator strength and selection rules for ligand field excitations change with external uniaxial pressure. We discuss the relation between the ligand field on $R^{3+}$ with the magnetism and dielectric properties of this compounds.

4:30PM T30.00007 THz magneto-optical study of multiferroic compound TbMnO3. URMAS NAGEL, D. HÜVONEN, T. RÖÖM, NICPB, Akadeemia tee 23, 12618 Tallinn, S.B. KIM, C.L. ZHANG, S.-W. CHEONG, Rutgers Center for Emergent Materials & Department of Physics and Astronomy, Rutgers University, NJ — We present results of magneto-optical absorption measurements in the THz region on multiferroic TbMnO3 in magnetic fields up to 12 T. The temperature range of our studies covers the paramagnetic phase (T > 42 K), the collinear incommensurate spin density wave phase of Mn$^{3+}$ with 2 spins (28 K < 42 K), the ferro-electric phase with incommensurate elliptic spin order (T < 28 K) and the phase where the magnetic moments of Tb are ordered, T < 7 K. It is known that in the FE phase the magnetic field B0 $\parallel$ a equal to 10.5 T flips the electric polarization from P $\parallel$ c to P $\parallel$ a. The polarization P is in the plane of elliptical spiral and perpendicular to spiral order vector, k $\parallel$ b in TbMnO3. It is expected that the selection rule for the electric-dipole active spin excitation in the spiral phase changes from E $\parallel$ a to E $\parallel$ c. Polarization-sensitive absorption measurements are performed to distinguish between magnetic- or electric-dipole active spin excitations, i.e. magnons or electromagnons, respectively, in the whole temperature and magnetic field range.

4:42PM T30.00008 Magneto-optical THz study in multiferroic Ni$_3$V$_2$O$_8$. DAN HÜVONEN, U. NAGEL, T. RÖÖM, NICPB, Akadeemia tee 23, 12618 Tallinn, Estonia, N. ROGADO, DuPont Central Research and Development, Experimental Station, Wilmington, Delaware 19880, R. CAVA, Dept. of Chem. and Princeton Mat. Inst., Princeton Univ., Princeton, NJ 08544 — We present results of absorption measurements in THz region, from 3 to 220 cm$^{-1}$, in multiferroic Ni$_3$V$_2$O$_8$ in magnetic fields up to 12 T and temperatures above 2 K. Ni$_3$V$_2$O$_8$ is a magnetic insulator with Ni$^{3+}$ spin-1 ions arranged in a kagome staircase lattice. The phase diagram of Ni$_3$V$_2$O$_8$ is complicated - ground state changes from paramagnetic (PM) to high temperature incommensurate (HTI) helical state, at 9.1 K in zero field. In low temperature incommensurate (LTI) phase below 6.3 K spontaneous electric polarization P appears along the b axis. P$_b$ can be suppressed by further cooling below 3.9 K or by application of external magnetic field. Low energy optical excitations are discussed for all low-T phases of Ni$_3$V$_2$O$_8$. Polarization sensitive absorption measurements are performed to distinguish between magnetoanisotropic spin excitations i.e. magnons and electromagnons. Different optical selection rules for magnon and electromagnon excitations enable us to search for evidence of the spin helix plane orientation and its changes at critical magnetic fields and temperatures.

1The support by the EstSF grants 6138 and 7011 is acknowledged.

1The support by the EstSF grants 6138 and 7011 is acknowledged.
4:54PM T30.00009 Evolution of magnetic exchange interactions in the multiferroic Mn$_{1-x}$Fe$_x$WO$_4$  , JAIME FERNANDEZ-BACA, FENG YE, RANDY FISHMAN, HERB MOOK, Oak Ridge National Laboratory, YIMING QIU, NCNR, NIST, R.P. CHAUDHURY, Y.-Q. WANG, B. LORENZ, C.W. CHU, University of Houston — The experimental investigation of the spin dynamical properties in the multiferroic material Mn$_{1-x}$Fe$_x$WO$_4$ is essential to the understanding of the interplay between the magnetic and ferroelectric phenomena. We have systematically studied the low temperature magnetic excitations in the Fe-doped Mn$_{1-x}$Fe$_x$WO$_4$. The spin wave dispersion relations in the commensurate (CM) phase are well described by a model that accounts for the magnetic exchange coupling of up to nine nearest neighbors. Our results indicate that these magnetic systems are highly frustrated and the CM spin structures result from the competing interactions. The evolution of the spin dynamics reveals the role of the magnetic impurities and the influence of Fe-doping to the multiferroic properties are discussed. This work was partially supported by Division of Scientific User Facilities of the Office of Basic Energy Sciences, U.S. DOE.

5:06PM T30.00010 Long-wavelength magnetic excitations in multiferroic BiFeO$_3$, D. TALBAYEV, J. G. GIGAX, A. J. TAYLOR, Los Alamos National Laboratory, SEONGSU LEE, S.-W. CHEONG, Rutgers University — Magnetic and lattice vibrations play a central role in the properties of multiferroics. This low-energy electrodynamic field can help unravel the fundamental interactions between magnetic and lattice degrees of freedom. BiFeO$_3$ is a multiferroic material with robust room temperature ferroelectricity and antiferromagnetism and promising technological potential. The interaction between the ferroelectric and antiferromagnetic order parameters leads to the modification of the isotropic Heisenberg-antiferromagnet ground state that becomes an incommensurate cycloid with a very long period. The cycloidal magnetic structure results in a complex spectrum of zero-wavevector magnetic excitations; these magnetic modes were detected using Raman scattering. Here, we report a far-infrared spectroscopic study of a BiFeO$_3$ single crystal. We detected magnetic resonances at energies close to those reported in the Raman spectroscopy studies. The magnetic character of these excitations is supported by their characteristic temperature dependence. We will discuss our results in the context of possible electric-dipole activity of the observed resonances.

5:18PM T30.00011 Low energy excitations in multiferroic Ca$_3$CoMnO$_6$ in the far infrared, ANDREI SUSHKOV, H.D. DREW, University of Maryland, Y.J. CHOI, H.T. YI, S. LEE, S.W. CHEONG, Rutgers University — Ferroelectricity was recently discovered in Ca$_3$CoMnO$_6$ (Y.J. Choi et al., PRL 100 (2008) 047601) which is a quasi 1D spin up-up-down-down system. We report the results of infrared (5-250 cm$^{-1}$) transmission study of multiferroic Ca$_3$CoMnO$_6$ as a function of temperature T (3-300 K) and magnetic field H (0-8 T). Two peaks are observed at and below T$_N$ = 17 K. Narrow peak at 35 cm$^{-1}$ is observed at low T and is identified as the ground state feature. This feature is suppressed with raising T or in magnetic field and the other broad feature at 25 cm$^{-1}$ emerges. Neither peak is split or shifted by magnetic field. We will discuss the possible origin of these two excitations.

Wednesday, March 18, 2009 2:30PM - 5:18PM –

Session T31 DMP GMAG: Focus Session: Magnetic, Electric, and Photo-Induced Magnetization Reversal

2:30PM T31.00001 Ultrafast magnetic imaging of nanostructures, YVES ACREMANN, SLAC — Today's technology advances into smaller and more complex structures for information processing. As structures get smaller, many processes of interest become faster as the propagation speed of excitations couple the length scale with the time scale. Microscopic techniques with a spatial resolution reaching the atomic level are being developed with very impressive success. On the other hand, time resolved techniques based on ultrafast laser systems allow us to explore processes on the femtosecond time scale. The focus of this talk is to unite the two worlds, the ultra-fast and the ultra-small. A powerful approach to time resolved microscopy is based on x-ray techniques. The wavelength of x-rays offers a spatial resolution in the nanometer range. Ultrafast x-ray techniques are currently being developed based on synchrotron sources as well as free electron lasers. The talk will demonstrate ultrafast microscopy techniques on imaging magnetization reversal dynamics in spin transfer devices.

2:30PM T31.00001 Ultrafast magnetic imaging of nanostructures

3:06PM T31.00002 Magnetization Dynamics of Magnetic Nano-Elements on Ultrafast Time Scales, J.P. DAVIS, J.A.J. BURGESS, University of Alberta, Z. LIU, R.D. SYDORA, M.R. FREEMAN, University of Alberta — Recently, our group has systematically studied the switching of a single permalloy nano-disk (160 nm diameter) between the vortex and quasi-single domain ground states as a function of applied bias field, including the observation of real-time switching at particular fields [1]. This was performed using the time-resolved magneto-optical Kerr effect (TR-MOKE), which allows dynamics to be studied on sub-nanosecond time scales. To accurately simulate the switching behavior, it was necessary to take into account the domed shape of the nano-disks, which result from the lift-off fabrication. Because of the sensitivity of the magnetization dynamics to the shape of the disks, we have begun fabrication of nano-disks using a shadow mask procedure [2] with a collimated deposition source under ultra-high vacuum (UHV) to produce high quality nano-elements. Magnetization dynamics of these UHV fabricated nano-disks will be discussed, with complementary scanning probe microscopy characterization of the disks.

3:06PM T31.00002 Magnetization Dynamics of Magnetic Nano-Elements on Ultrafast Time Scales

3:18PM T31.00003 Ultrafast switching of a nanomagnet by a combined in-plane and out-of-plane polarized spin-current pulse, OUKJAEE LEE, V.S. PRIBIAG, P.M. BRAGANCA, P.G. GOWTHAM, E.M. RYAN, D.C. RALPH, R.A. BUHRMAN, Applied and Engineering Physics, Cornell University — For fast write operation of a spin-torque (ST) magnetic storage device, the exertion of a strong initial torque can switch the nanomagnet moment without the help of the thermal fluctuations. Use of an out-of-plane polarized reference layer can very quickly excite large free layer motion but reliable reversal requires precise ST pulse timing. The combination of strong in-plane and out-of-plane polarized spin currents can substantially relax this pulse-timing requirement. We have fabricated CPP spin-valve devices that incorporate both an out-of-plane polarizer, and an in-plane polarizer to quickly excite and reverse the moment of an in-plane polarized free layer. For pulse currents ranging between 100ps – 10ns, the reversal speeds are notably faster and much less thermally distributed than for a conventional spin-valve with the same pulse current amplitude. We will discuss the details of the short-pulse behavior of these device structures and the optimization of this approach for high-speed magnetic memory.
3:30PM T31.00004 Total angular momentum conservation in laser-induced femtosecond magnetism\textsuperscript{1}. GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, Indiana 47809, YIHUA BAI, Center for Instruction, Research and Teaching, Indiana State University, Terre Haute, Indiana 47809, THOMAS F. GEORGE, Office of the Chancellor and Departments of Chemistry & Biochemistry and Physics & Astronomy University of Missouri-St. Louis — Spin momentum is not a classical quantity\textsuperscript{1,2}. It is unclear how the conservation law affects spin momentum change in laser-induced femtosecond magnetization\textsuperscript{3}. In solids, the rotational symmetry is lifted by the translational symmetry, and the spin and orbital momenta components of different total angular momentum mix to some extent. This mixing is the origin of the time-dependent total angular momentum in experiments. The remaining unmixed portion accounts for an extra spin change in three independent circularly-polarized laser experiments by G. P. Zhang et al., Phys. Rev. Lett. 85, 012407 (2000). \textsuperscript{2}G. P. Zhang and T. F. George, Phys. Rev. B 78, 052407 (2008). \textsuperscript{3}G. P. Zhang and W. Höhner, Phys. Rev. Lett. 103, 07B113 (2008).

\textsuperscript{1}Supported by DOE under Contract No. DE-FG02-06ER46304, Promising Scholars grant, and NERSC at LBNL under Contract No. DE-AC02-05CH11231.

3:42PM T31.00005 Evolution of magnetic states in ferromagnetic nanorings in an applied azimuthal field\textsuperscript{1}. ABBY GOLDMAN, KATHERINE AIDALA, Mount Holyoke College, TIANYU YANG, MARK TUOMINEN, University of Massachusetts, Amherst — Ferromagnetic nanorings form unique magnetic states that hold tremendous potential for maximizing data storage densities. One such state is the closed-flux vortex state, in which the magnetic field is completely enclosed within the ring, thus minimizing the magnetostatic energy, but also keeping the exchange energy low as adjacent magnetic moments are mostly aligned. A natural way to generate this state is through an external azimuthal field, as if from a current carrying wire passing through the center of the ring. We perform micromagnetic simulations to investigate the evolution of magnetic states in an external azimuthal field. For some applied current, the chirality of the ring will reverse, often into an intermediate state that evolves into a perfect vortex at higher current. Thin, wide rings have significantly lower switching currents than thick, narrow rings. We examine the dependence of the switching current and intermediate states on geometric properties such as the diameter, thickness, asymmetry and width of the ring.

\textsuperscript{1}This work was supported at Mount Holyoke in part by NSF NSEC materials was supported by the US DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

3:54PM T31.00006 Polarity reversal of magnetic vortex core by in-plane non-resonant pulsed magnetic field\textsuperscript{1}. XUEMEI CHENG, DAVID KEAVNEY, Argonne National Laboratory, KRISTEN BUCHANAN, Colorado State University — Magnetic vortices have been of great interest because of their potential applications in non-volatile data storage. Recently, Van Waeyenberge et al. demonstrated vortex core reversal in permalloy squares using an in-plane r.f. excitation field with the frequency close to the translational-mode eigenfrequency. In this work we report polarity reversal of magnetic vortex core by non-resonant in-plane field pulses. The core polarity was first determined by watching the sense of vortex core gyration in a 6 micron permalloy disk imaged by time-resolved x-ray photoemission electron microscopy (TR-PEEM) with 1mT excitation field pulses. After the waveguide was pulsed at 5mT, we determined core polarity at 1mT again. We also found that the core polarity can be switched back and forth by pulsing at 5mT. The micromagnetic simulations and TR-PEEM images confirm that when the core is displaced beyond 25% of disk radius, distortions of the core region occur, promoting a transient domain state involving a complex cross-tie wall, and subsequent reversal of the core polarity.

\textsuperscript{1}Use of the Advanced Photon Source and Center for Nanoscale Materials was supported by the US DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

4:06PM T31.00007 Hybridization of quantum spin waves in small structures, VALENTYN NOVOSAD, Argonne National Lab, S.T. CHUI, University of Delaware, SAM BADER, Argonne National Lab — We apply the Holstein-Primakoff and Bogoliubov transformations to compute the spin wave states of small magnetic structures including the effect of the dipolar interaction. We found that as the film gets thicker, states with a significant q=0 component are hybridized with states with higher Fourier components. In the presence of a static magnetic field opposite to the magnetization direction, surface states that are responsible for magnetization reversal are coupled to the extended states. The response function is increased by an order of magnitude. This suggests an intriguing scenario for assisted switching of the magnetization with an additional external a.c. field.

4:18PM T31.00008 Electric field-induced modification of magnetism in thin CoPd films.\textsuperscript{1}. MIKHAIL ZHERNENKOV, MICHAEL FITZSIMMONS, JERZY CHLISTUNOFF, JAREK MAJEWSKI, LANL, IOAN TUDOSA, ERIC FULLERTON, UCSD — Recently, M. Weisheit et al., Science 315, 349 (2007) reported modification of magnetic properties of thin-film ferromagnets by applying a large electric field at the surface of a ferromagnet. For an applied voltage of -0.6 V, the coercivities of 20 Å thick FePt and FePd films were changed by -4.5 and +1%, respectively. Here, we report polarized neutron reflectometry measurements of the magnetization depth profile of a 180 Å thick Co$_{50}$Pd$_{50}$ film immersed in an electrolyte as a function of applied electric field in an external magnetic field. The measurements were done at two values of applied electric potential of -0.6 volts and -1.2 volts and at zero volts (open-circuit potential). The applied magnetic field was 3 kG. We found a linear increase of the film magnetization with electric field. The change of magnetization occurred in the region of the film within 72 Å of the electrolyte/Co$_{50}$Pd$_{50}$ interface. The magnetization of the top part of the layer is increased by 2% (-0.6 V) and 3.6% (-1.2 V) compared to the open circuit potential result.

\textsuperscript{1}This work was supported by DOE.

4:30PM T31.00009 Electric-field-driven spin resonance of a Mn dopant in GaAs, V.R. POVILUS, Department of Physics and Astronomy University of Iowa, J.-M. TANG, Department of Physics University of New Hampshire, M.E. FLATTE, Department of Physics and Astronomy University of Iowa — All-electric manipulation of the ground-state spin system of a Mn dopant in GaAs using a static electric field in combination with a transverse dynamic electric field requires careful positioning of two gates on the nanoscale\textsuperscript{1}. Here we propose a method of efficiently controlling the spin of a Mn dopant using parallel static and dynamic electric fields, but adding a small static magnetic field. In a scalable geometry this would permit full control of the ground-state J=1 spin of a Mn dopant using a single electric gate. The energy states and eigenfunctions of the Mn dopant system under the influence of both an electric and magnetic field cannot be simply described using an effective electric-field-dependent g tensor, as would be done in g tensor modulation resonance\textsuperscript{2}. However, the dynamical equations for the spin can be numerically solved and exhibits high-visiblity Rabi oscillations. For example, with a static electric field of 500 V/cm, a dynamic electric field of 300 V/cm with frequency 9.1 GHz, and a magnetic field of 0.1 Tesla, all oriented in the [113] direction, the Rabi oscillation period is 2.7 ns.


4:42PM T31.00010 ABSTRACT WITHDRAWN —
4:54PM T31.00011 Photoinduced Magnetism of Ternary Transition Metal Prussian Blue Analogos, D.M. PAJEROWSKI, M.W. MEISEL, Dept. Phys., Univ. Florida, J.E. GARDNER, D.R. TALHAM, Dept. Chem., Univ. Florida — The magnetism of Prussian blue analog materials (PBAs) can be tuned with external stimuli such as temperature, pressure, and light. Recently, novel effects have been seen in PBAs with substitutionally mixed ternary and quaternary transition metals, rather than the usual binary analogs. One noteworthy material we have studied is a Na$_{8}$Ni$_{1-x}$Co$_{x}$[Fe(CN)$_{6}$]$_{3}$·$n$H$_{2}$O powder, which can show either a photoinduced increase or decrease in magnetization depending upon the Ni substitution, the applied magnetic field, and the temperature. This result is the first example of a photoinduced decrease in magnetization while generating new spins via a charge transfer induced spin transition (CTIST) in a bulk material. Constrastingly, the photodecrease observed in PBA binary thin films has different microscopic origins [1-2]. Insight into the underlying mechanisms can be obtained by using mean field models, which qualitatively reproduce the experimental data. SQUID, magnetometer, FT-IR, TEM, and EDS data will be presented.

1This work was supported, in part, by NSF DMR-0701400 (MWM) and NSF DMR-0453362 (DRT).

5:06PM T31.00012 Bismuth in strong magnetic fields: unconventional Zeeman coupling and correlation effects, JASON ALICEA, Caltech, LEON BALENTS, KITP — Recent experiments on bismuth have uncovered remarkably rich magnetization structure at fields well beyond the regime in which all carriers are expected to reside in the lowest Landau level. Motivated by these findings, we start from a microscopic tight-binding model and derive a low-energy Hamiltonian for the holes and three Dirac electrons pockets in bismuth. We find that an unconventional electron Zeeman effect, overlooked previously, suppresses the quantum limit for the electrons dramatically, giving rise to the observed anomalous magnetization hysteresis was observed. Here we find instabilities towards both charge density wave and Wigner crystal phases, and propose that hysteresis arises from a first-order transition out of the latter.

Wednesday, March 18, 2009 2:30PM - 5:30PM –
Session T32 GMAG DMP FIAP: Focus Session: Gilbert Damping and Non-local Spin Injection

2:30PM T32.00001 Anisotropic Damping in Single-Crystalline Ni/MgO(001) studied by the Time-Resolved Magneto-Optical Kerr effect (TR-MOKE), KEVIN SMITH, A. LUKASZEW, J. SKUZA, C. CLAVERO, K. YANG, A. REILLY, G. LÜPKE, William and Mary — The damping behavior of uniform spin precession in single-crystalline Ni/MgO(001) of various thicknesses from t = 10 nm to t = 60 nm is investigated in the time domain using TR-MOKE over a wide range of external field parameters and temperatures. Planar measurements indicate that the effective Gilbert damping parameter, $\alpha_{\text{eff}}$, is coupled to the magnetocrystalline anisotropy, as $\alpha_{\text{eff}}$ ranges from 0.05 near the hard axis to 0.10 near the easy axis. Previous experiments by other groups using FMR [1] and TR-MOKE on polycrystalline samples [2] have placed the intrinsic value of the damping at 0.045. When the field is applied normal to the film surface, $\alpha_{\text{eff}}$ increases to as high as 0.3 when the angle of the magnetization, as measured from the film plane, approaches 45 degrees from the easy axis of the film.


2:42PM T32.00002 Scattering Theory of Gilbert Damping, ARNE BRATAAS, Norwegian University of Science and Technology, Department of Physics, NO-7491 Trondheim, Norway, YAROSLAV TSERKOVNYAK, University of California, Los Angeles, Department of Physics and Astronomy, CA 90095, USA, GERRIT E.W. BAUER, Delft University of Technology, Kavli Institute of Nanoscience, Lorentzweg 1, 2628 C J Delft, The Netherlands — Magnetization relaxation is a collective many-body phenomenon that remains intriguing despite decades of theoretical and experimental investigations. It is important in topics of current interest since it determines the magnetization dynamics in magnetic memory devices and state-of-the-art magnetoelectronics experiments on Co-based films. In this talk, we discuss magnetization dynamics of a single domain ferromagnet in contact with a thermal bath by scattering theory. We recover the Landau-Lifshitz-Gilbert equation and express the Gilbert damping tensor in terms of the scattering matrix [2]. Dissipation of magnetic energy equals energy current pumped out of the system by the time-dependent magnetization, with separable spin-relaxation induced bulk and spin-pumping generated interface contributions. In linear response, our scattering theory for the Gilbert damping tensor is equivalent with the Kubo formalism [1] M. Stiles and J. Miltat, Top. Appl. Phys. 101, 225 (2006), and references therein. [2] A. Brataas, Y. Tserkovnyak, and G. E. W. Bauer, Phys. Rev. Lett. 101, 037207 (2005).

2:54PM T32.00003 Physical damping processes in Co-Cr granular films, SANGITA KALARICKAL, PAWOL KRIVOSIK, NAM MO, CARL PATTON, Colorado State University, Fort Collins, CO, STELLA WU, Seagate Technology, Fremont, CA — Recent ferromagnetic resonance (FMR) results on metallic ferromagnetic alloy films have shown that a simple one parameter Gilbert damping description is inadequate for most systems. New FMR results have been obtained on Co-Cr granular films with the columnar microstructure amenable to perpendicular media applications. The nominal 17.3 GHz FMR field and linewidth vs. the out-of-plane field angle was measured and analyzed for a 16 nm thick granular film with a relatively low effective anisotropy field of 1 kOe and a nominal grain size of 8 nm or so. The analysis reveals a three component linewidth comprised of a small Gilbert term with an $\alpha$-value of 0.003 that is consistent with intrinsic processes, a large two magnon term that derives from the grain-to-grain anisotropy variations, and an inhomogeneity broadening term due to anisotropy dispersion and grain size variations.

1Supported in part by the INSIC EHDR program and Seagate Technology.

2On leave from Slovak University of Technology, Bratislava, Slovak Republic.

3Now at Tyco Electronics, Reno, NV

3:06PM T32.00004 Effect of rapid thermal annealing on ferromagnetic resonance line width of CoFeB thin films, YAPING ZHANG, XIN FAN, WEIGANG WANG, XING CHEN, Department of Physics & Astronomy University of Delaware, CHAOYING NI, Department of Materials Science University of Delaware, RONG CAO, JOHN XIAO, Department of Physics & Astronomy University of Delaware — Magnetization dynamics has attracted much attention recently due to their implication on magnetic recording and storage applications. CoFeB is one of most common magnetic layers used in MgO based magnetic tunnel junctions (MTJs). Unlike traditional thermal treatments, a giant Tunneling Magnetoresistance can be archived by rapid thermal annealing (RTA) [1]. We show the effect of RTA on magnetization dynamics. CoFeB thin film, subjected to RTA at 380 °C for various time, was investigated by ferromagnetic resonance (FMR) measurement. It is found that FMR linewidth reaches a minimum at 60 second annealing, after which the linewidth increases with annealing time. A clear trend of decreasing of uniaxial anisotropy and increasing of cubic anisotropy with annealing time indicates that competition between these anisotropies plays an important role in linewidth evolution. [1] WG. Wang et al., Appl. Phys. Lett. 92, 152501 (2008).
3:18PM T32.00005 Calculation of intrinsic damping in half metals, CHUNSHENG LIU, CLAUDIA K.A. MEWES, MAIRBEK CHSHIEV, TIM MEWES, WILLIAM H. BUTLER, MINT Center, University of Alabama, Tuscaloosa, AL — The extended Hückel tight binding method in combination with Kambersky’s torque correlation model [1] is used to calculate the precessional magnetization relaxation in half-metallic systems. In Kambersky’s model damping is described by a combination of spin-flip excitations and orbital excitations. An analytical expression of the transition matrix element which represents scattering events within a single band (intra-band) and between different bands (inter-band) respectively [2] can be obtained within the TB scheme, which enables a better understanding of the damping mechanisms in half-metallic structures. Due to the absence of spin-flip scattering in non-magnetic systems, the Gilbert damping rate of half-metals is expected to be much smaller than that of metals. Using this approach we calculated the damping for different half-metallic structures. The minimum intrinsic relaxation rate \( \lambda \) was calculated to be, 3.2 MHz, 1.1 MHz, 0.13 MHz, for the Heusler structures Co2MnGe, Co2MnSi and the Rutile structure CrO2 respectively. The damping rates for these half-metallic materials are much lower than that of bcc Fe, as we anticipated from the analytical analysis. References: [1] V. Kambersky, Czech. J. Phys. B 26, 1366 (1976). [2] K. Gilmore, Y.U. Izdebera and M.D. Stiles, Phys. Rev. Lett. 99, 027204 (2007).

3:30PM T32.00006 Unidirectional Damping in Exchange Biased Systems1, MATTHEW BRADFORD, HWACHOL LEE, ERIC EDWARDS, ZEENATH TADISINA, CLAUDIA MEWES, SUBHAJIT GUPTA, TIM MEWES, The University of Alabama — We report on the investigation of the angular dependence of the damping parameter in thin film NiFe, exchange biased by a layer of FeMn. By using a broadband ferromagnetic resonance technique (shorted waveguide), the resonant field and linewidth were determined as a function of the in-plane angle and the microwave frequency. We find that the effective damping parameter, as extracted from the frequency dependent linewidth data, shows a unidirectional anisotropy, displaying a sinusoidal behavior with respect to the in-plane angle. The effective damping parameter is minimal when the field during FMR measurements is applied parallel to the exchange bias direction and maximal for parallel alignment. These experiments in conjunction with thickness dependent measurements suggest that uncompensated spins at the ferromagnet/antiferromagnet interface are responsible for the increased magnetization relaxation observed in these structures.

1We gratefully acknowledge support from the NSF (DMR 0804243).

3:42PM T32.00007 The origin of intrinsic Gilbert damping1, MARK C. HICKEY, JAGADEESH S. MOODER, MIT — The damping of magnetization, represented by the rate at which it relaxes to equilibrium, is successfully modeled as a phenomenological extension in the Landau-Lifschitz-Gilbert equation. This is the damping term known as Gilbert damping and its direction is given by the vector product of the magnetization and its time derivative. Here we derive the Gilbert term from first principles by a non-relativistic expansion of the Dirac equation. We find that the Gilbert term arises when one calculates the spin observable in the presence of the full spin-orbital coupling terms, while recognizing magnetization and its time derivative. Here we derive the Gilbert term from first principles by a non-relativistic expansion of the Dirac equation. We find that the Gilbert term arises when one calculates the spin observable in the presence of the full spin-orbital coupling terms, while recognizing magnetization and its time derivative. The Gilbert damping rate is proportional to the dimensionless parameter \( \beta \) that can be applied to real materials. We also discuss the consequences of \( \alpha \) and \( \beta \) in out-of-equilibrium superconductors viewed as easy-plane ferromagnets in particle-hole space.

3:54PM T32.00008 Theory of Magnetization Relaxation in Conducting Ferromagnets, ION GARATE, University of Texas at Austin — The advent of technologically promising spintronics devices has revived efforts to achieve a microscopic understanding of magnetization damping in magnetic metals and semiconductors. In absence of an electric current, magnetization relaxation is described by the Gilbert parameter \( \alpha \), whose quantitative prediction relies on electronic structure calculations that treat disorder in an approximate fashion. We assess the reliability of these studies by using simple models where disorder may be treated exactly. Transport currents modify the magnetization damping. We associate this change with the non-adiabatic spin transfer torque, which is characterized by a dimensionless parameter \( \beta \). We derive a concise analytical expression for \( \beta \) that can be applied to real materials. We also discuss the counterparts of \( \alpha \) and \( \beta \) in out-of-equilibrium superconductors viewed as easy-plane ferromagnets in particle-hole space.

4:00PM T32.00009 Nonlocal Spin Valves With Very Short Injector Detector Distances, ANDREW MCCALLUM, MARK JOHNSON, Naval Research Laboratory — Nonlocal spin valves with a center to center distance of 42 nm between spin injector and detector have been fabricated. This distance is much less than the injector detector spacing in previously made nonlocal spin valves and is much shorter than the spin diffusion length of the Cu used as a channel. Nonlocal resistance changes of up to 2.6 m\( \Omega \) were seen in these devices at room temperature. From this data it was determined that the effective spin polarization of the ferromagnetic interfaces is between 4.5% and 5.9% at room temperature. The nonlocal resistance changes of these devices are much less sensitive to changes in temperature, as determined by measurements at liquid nitrogen temperature, than nonlocal spin valves with longer injector detector distances.

4:42PM T32.00010 Temperature dependence of the non-local spin signal in Cu-based lateral spin-valves, M.J. ERICKSON, C. LEIGHTON, P.A. CROWELL, University of Minnesota — We report on measurements of the \( T \) dependence of the non-local spin signal in lateral metal spin valves, focusing on the limit of transparent ferromagnet (FM) / normal metal (Cu) interfaces. Devices with channel width 250 nm and contact widths \( \approx 100 \) nm (NiFeFe\, or Co) were fabricated using in-situ shadow masking. We employed high purity sources in UHV, enabling one-shot deposition without air exposure of the interface. Multiple contact separations (250 – 800 nm) were fabricated on a single substrate to facilitate measurement of the spin diffusion length (\( \lambda_s \)). NiFe/Cu devices with 250 nm contact separation show a maximum non-local transresistance of 420 \( \mu \Omega \). Analysis of Hanle effect measurements yields spin lifetimes \( \approx 8 \) ps at low \( T \) which compare well to those extracted from the measured \( \lambda_s \) (300 nm) and resistivity (1.5 \( \mu \Omega \cdot \text{cm} \)), demonstrating consistency of our analysis. We observe a qualitatively different \( T \) dependence of the non-local signal depending on the relative sizes of the contact separation and \( \lambda_s \). When the separation becomes comparable to \( \lambda_s \), we observe a maximum in the non-local spin signal at 35 – 85 K, with strongly thickness dependent magnitude. These measurements of spin lifetime, resistivity, and \( \lambda_s \) vs \( T \) allow a quantitative comparison with the conductivity mismatch model. Work supported by the NSF MRSEC program.

4:54PM T32.00011 Bias-independent spin signals in a tunnel-junction-based non-local spin valve1, XIAOJUN WANG, HAN ZOU, L.E. OCOLA, R. DIVAN, YI JI2 — A pure spin current can be generated in the non-magnetic component of a non-local spin valve (NLSV). It has been demonstrated recently that the pure spin current can be used for spin transfer torque and spin-Hall effects. A high spin current density is desirable for realizing these effects, and therefore a large d.c. bias current will be applied. It is essential to maintain high degree of spin polarization at a high bias current. It has been previously reported that the spin polarization decreases drastically in a tunnel-junction-based CoFe/Au/NiFe NLSV. The goal of this study is to investigate the dependence of spin signals upon a d.c. bias current in tunnel-junction-based Co/Cu/Co NLSV’s. Submicron Co/Cu/Co NLSV’s are fabricated by e-beam lithography combined with angle deposition. A layer of 2 nm AlOx is deposited at the Co/Cu interface to form a tunnel barrier. A spin signal > 1m\( \Omega \) is observed at room temperature (RT). A d.c. current up to 1.0mA is applied at both 4.2 K and RT. No change of spin signal is observed for an injection current density > 10\( ^4 \) A/cm\(^2 \).

1This work is supported by U.S. DOE Grant No. DE-FG02-07ER46374. Use of the Center for Nanoscale Materials was supported by the U.S. DOE under contract No. DE-AC02-06CH11357.

2yji@physics.udel.edu
5:06PM T32.00012 Separating the Contributions of Spin Injection Efficiency and Spin Diffusion Length in Non Local Spin Valves1, MIKHAIL EREKHINSKY, FELIX CASANOVA, AMOS SHARONI, IVAN K. SCHULLER, University of California, San Diego — Non Local Spin Valves (NLSV) are unique devices which permit studies of spin transport related phenomena at the nanoscale. Two important parameters determine the signal in NLSV: a) the effective polarization of injected current from the ferromagnet (FM) through the interface, and b) the spin diffusion length of the non-magnetic metal (NM). We performed a systematic study of the NLSV signal for different device lengths as a function of NM thickness, composition and temperature. By fitting the near-exponential decay of the signal with distance we can separate the effects of polarization and NM spin diffusion length. We will discuss the contributions of surface effects on NM spin diffusion length, and FM/NM interface on efficiency of injection. In addition, we show the importance of adjacent FM electrodes in a multi-terminal spintronic device.

1This work was supported by US-DOE

5:18PM T32.00013 Control of Spin Injection by DC Current in Transparent Lateral Spin Valves1, AMOS SHARONI, FELIX CASANOVA, MIKHAIL EREKHINSKY, IVAN K. SCHULLER, UC San Diego — Lateral spin valves can be classified according to the type of interfaces (tunnel or transparent) between the ferromagnetic electrodes and the normal material. The tunnel barrier yields a large spin signal, but the maximum spin-polarized current was reported to decrease strongly with applied bias. In transparent interfaces the maximum current density through the interface is much larger, which is beneficial for some applications, but the effect on spin signal was not measured. To address this issue, we prepared metallic lateral spin valves with excellent transparent interfaces. In addition, instead of AC lock-in techniques commonly used to measure these devices, we perform DC measurements, which enables us to measure directly the effects of the current direction and magnitude on the spin signal. We compared the injection of majority spins from the ferromagnet into a non-magnetic metal (NM) with the reversed process where minority carriers are left in the NM. We were also able to study the effect of joule heating and identified the origin of voltage backgrounds usually observed in these devices.

1Work supported by DOE

Wednesday, March 18, 2009 2:30PM - 5:30PM –
Session T33 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors XI: Penetration Depth and Magnetic Anisotropy 403

2:30PM T33.00001 Temperature Dependence of the Penetration Depth of LaFePO from Scanning SQUID Susceptometry, CLIFFIRD HICKS, THOMAS LIPPMAN, Geballe Laboratory for Advanced Materials, Stanford University, MARTIN HUBER, Departments of Physics and Electrical Engineering, University of Colorado at Boulder, JAMES ANALYTIS, JUIN-HAW CHU, IAN FISHER, KATHRYN MOLER, Geballe Laboratory for Advanced Materials, Stanford University — We use a scanning SQUID susceptometer to measure locally the temperature dependence of the penetration depth of the superconductor LaFePO. We observe a linear temperature dependence down to 850 mK, with a slope that varies with position on the sample. This is in contrast to recent measurements on the related iron arsenide family of superconductors, which indicate fully-gapped superconductivity. We also report on our ability to measure Tc locally, and observe local regions with weak superconductivity at temperatures well above the dominant Tc.

2:42PM T33.00002 Broadband microwave absorption of Fe-based superconductors, JAKE BOBOWSKI, PINDER DOSANJH, JAMES DAY, DOUG BONN, WALTER HARDY, Department of Physics and Astronomy, University of British Columbia — Preliminary microwave measurements of the penetration depth in single crystals of the hole-doped iron-based superconductor Ba1−xKxFe2As2, using cavity perturbation and ac susceptometry, have been performed by our group. These results hint at a gap with nodes plus the presence of scattering. As a complement to these techniques, we have also undertaken broadband microwave absorption (i.e., surface resistance) measurements on the same pnictide samples. Our initial results of the microwave conductivity are consistent with a system possessing a finite density of states at low temperature due to impurity scattering which then evolves with temperature above about 5 K.

2:54PM T33.00003 Lower Critical Fields and the Anisotropy in PrFeAsO1−y Single Crystals, RYUJI OKAZAKI, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, MARCIN KONCZYKOWSKI, C.J. VAN DER BEEK, Laboratoire des Solides Irrades, Ecole Polytechnique, 91128, Palaiseau, France, TOMONARI KATO, KEN-ICHIRO HASHIMOTO, MASAAKI SHIMOZAWA, HIROAKI SHISIDO, MINORU YAMASHITA, TAKASADA SHIBAUCHI, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, MOTOYUKI ISHIKADO, SHIN-ICHI SHAMOTO, Quantum Beam Science Directorate, JAEA, Tokai, Naka, Ibaraki 319-1195, Japan, HIJIRI KITO, AKIRA IYO, HIROSHI EISAKI, Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto 606-8502, Japan, Laboratoire des Solides Irrades, Ecole Polytechnique, 91128, Palaiseau, France — By utilizing miniature Hall-sensor array, we evaluated the lower critical fields Hc1 in Fe-based oxipnictide PrFeAsO1−y, single crystals for H||c and H||ab-planes. The temperature dependence of Hc1 for H||c is well scaled by the in-plane penetration depth and is consistent with a full-gap superconducting state. The anisotropy of penetration depths at low temperatures is estimated to be ≃ 3, which is much smaller than that of coherence lengths. This indicates the multiband superconductivity, in which the active band for the superconductivity is more anisotropic.

3:06PM T33.00004 Temperature Dependent Anisotropy of Oxypnictide Superconductors Studied by Torque Magnetometry, STEPHEN WEYENETH, Physics Institute, University of Zurich, 8057 Zurich, Switzerland, RO-MAN PUZNIAK, Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland, NIKOLAI D. ZHIGADLO, SERGIY KATRICHYK, ZBIGNIEW BUKOWSKI, JANUSZ KARPINSKI, Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland, URS MOSELE, STEFAN KOHOUT, JOSEF ROOS, HUGO KELLER, Physics Institute, University of Zurich, 8057 Zurich, Switzerland — Single crystals of different oxypnictide superconductors of the family ReFeAsO1−x−Fy (Re = Sm, Nd, Pr) with various carrier dopings and with masses m ≃ 100 mg have been investigated by means of torque magnetometry. We present most recent data, obtained by using highly sensitive piezoresistive torque sensors from which the superconducting anisotropy parameter γ and the in-plane magnetic penetration depth λc were extracted. As an important result γ was found to increase strongly as the temperature is decreased from Tc down to low temperatures. This unconventional temperature dependence of γ is similar to that observed in the two-band superconductor MgB2 and cannot be explained within the classical Ginzburg-Landau model. This scenario strongly suggests a new multi-band mechanism in the novel class of oxypnictide high-temperature superconductors.
3:18PM T33.00005 Magnetic penetration depth and critical current density in aligned grains of NdFeAsO(F)1, YURI L. ZUEV, E. D. SPECHT, D. K. CHRISTEN, Oak Ridge National Laboratory, J. R. THOMPSON, Dept. of Physics, University of Tennessee, and Oak Ridge National Laboratory, R. JIN, B. C. SALES, A. SEPAT, M. A. McGUIRE, D. G. MANDRUS, Oak Ridge National Laboratory — We have prepared a powder sample of NdFeAsO(F), where most crystallite particles are aligned with their c-axis along a common direction. We have measured magnetic penetration depth and a critical current density in the base-plane. The penetration depth shows a fully gapped superconducting state with two energy gaps, one roughly twice as large as the other. The in-plane critical current density is as high as several MA/cm² at low temperatures, zero field, which may be promising for applications.

1Research sponsored by the DOE Division of Materials Sciences and Engineering

3:30PM T33.00006 Low temperature penetration depth of Fe-based superconductors, JAMES DAY, BRAD RAMSHAW, JAKE BOBOWSKI, PINDER DOSANJH, DOUG BONN, WALTER HARDY, Department of Physics and Astronomy, University of British Columbia — The recent discovery of superconductivity in layered iron-based pnictide compounds has generated levels of excitement comparable to the early days of the copper-based oxide superconductors. While connections may be drawn between the cuprates and the pnictides, there exist important differences between the two materials. We report high-precision microwave measurements of the penetration depth in single crystals of the hole-doped iron-based superconductor Bax1−xK2Fe2As2. Using cavity perturbation techniques in conjunction with ac susceptometry, we find that the low temperature penetration depth does not fit well to a simple s-wave model. Furthermore, our initial results suggest that the temperature dependence of the superfluid density is consistent with a gap with nodes plus the presence of scattering.

3:42PM T33.00007 Penetration Depth and Quasiparticle Conductivity in Iron-based High-Temperature Superconductors, KEN-ICHIRO HASHIMOTO, TAKASADA SHIBAUCHI, TOMONARI KATO, KOSUKE IKADA, RYUJI OKAZAKI, HIROSKI SHISHIDO, Department of Physics, Kyoto University, C.J. VAN DER BEEK, M. KONCZYKOWSKI, Ecole Polytechnique, HIJIRI KITO, AKIRA IYO, HIROSHI EISAKI, AIST, MOTÖYUKI ISHIKADO, SHIN-ICHI SHAMOTÔ, JAE, H. TAKEYA, K. HIRATA, NIMS, SHIGERU KASAHARA, TAKAHITO TERAISHIMA, Research Center for Low Temperature and Materials Sciences, Kyoto University, YUIJI MATSUDA, Department of Physics, Kyoto University — We measure the in-plane penetration depth and the quasiparticle conductivity in the newly discovered Fe-based high-temperature superconductors PrFeAsO1−x[1] and Ba1−xK2Fe2As2[2], using a sensitive superconducting resonator. We show that the penetration depth exhibits a very flat behavior at low temperatures in both compounds, which indicates that the superconducting gap opens up all over the Fermi surface. The temperature dependence of the superfluid density is well fitted with the two gap model, suggesting the multi-gap nature of superconductivity in this system. Moreover, the observed large enhancement of the quasiparticle conductivity suggests a suppression of the quasiparticle scattering, reminiscent of the superconductors in strongly correlated electronic systems.[1] K. Hashimoto et al., arXiv:0806.3149., [2] K. Hashimoto et al., arXiv:0810.3506.

3:54PM T33.00008 London Penetration Depth in Single Crystals of Nd(Fe,Co)As(O,F) Superconductors, H. KIM, C. MARTIN, R.T. GORDON, M.A. TANATAR, M.E. TILLMAN, S. KIM, S.L. BUD’KO, P.C. CANFIELD, R. PROZOROV — Iron arsenide superconductors, with the general formula RFeAsO−x[1] (R=Nd,Sm,Pr,Gd), exhibit the highest transition temperatures among the compounds of the pnictide family, in excess of 50 K. London penetration depth measurements performed on single crystals, grown under high pressure with nominal fluorine content x=0.1, have revealed a nodeless superconducting state with a modestly anisotropic gap[1]. Since doping is one of the most efficient ways to perturb the superconductivity, we explore here the evolution of the London penetration depth with doping, achieved by F substitution on O sites and by Co substitution on Fe sites. Notable differences in the superconducting transition temperatures for the two sets of crystals suggests the importance of impurity scattering for quasiparticles, which is characteristic of a superconducting gap function possessing some type of nodal structure. The overall change in the superfluid density as a function of doping will be discussed. R. T. Gordon et al. arXiv:0807.0876

4:06PM T33.00009 Co-concentration dependence of the London penetration depth in single crystals of Ba(Fe1−x,Co)xAs2, R. T. GORDON, C. MARTIN, H. KIM, M.A. TANATAR, N. NI, S.L. BUD’KO, P.C. CANFIELD, J. SCHMALIAN, R. PROZOROV, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — The in-plane London penetration depth, λab(T), has been measured in single crystals of Ba(Fe1−x,Co)xAs2 for several values of x using a tunnel diode resonator (TDR) technique. The low temperature behavior of the variation of the penetration depth follows a clear power law behavior, Δλ(T) ∝ T−n, for all measured Co concentrations with n varying between 2 on the underdoped side to about 2.5 at the optimal doping. This non-exponential behavior in Δλ indicates the existence of a significant number of superconducting quasiparticles, which is characteristic of a superconducting gap function possessing some type of nodal structure. The overall change in the superfluid density as a function of doping will be discussed. R. T. Gordon et al. arXiv:0810.2295 (2008).

4:18PM T33.00010 Magnetic force microscopy study of a Ba0.55K0.45Fe2As2 single crystal: Local penetration depth and flux pinning, LAN LUAN, OPHIR M. AUSLAENDER, KATHRYN A. MOLER, JAMES G. ANALYTIS, JIUN-HAW CHU, IAN R. FISHER, Stanford University — We use a magnetic force microscope (MFM) to study both the penetration depth (λab) and flux pinning in the iron-pnictide superconductor Ba0.10K0.45Fe2As2 by imaging and manipulating vortices. We observe the same regular signature from all vortices in a 50μm × 50μm field of view, implying lattices. While inhomogeneity of the superfluid density down to the sub-micron scale, Quantitative analysis of images between vortices and of the Meissner repulsion of the magnetic tip from the sample gives the temperature-induced change of λab and an estimate for its absolute value. We detect no long-range order in the vortex positions, suggesting the absence of correlated pinning in the material. We measure the force required to depin individual vortices and the force required to drag them across the entire sample. This allows us to characterize the pinning potential in the material and its distribution as well as to set bounds on the local critical current.

4:30PM T33.00011 Evidence for Two Energy Gaps in Superconducting Ba0.6K0.4Fe2As2 Single Crystals and Breakdown of the Uemura Plot, CONG REN, ZHAO-SHENG WANG, HUI-QIANG CHAI, HU, YUAN HUANG, LEI SHAN, HAI-HU WEN, National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, CAS, NATIONAL LABORATORY FOR SUPERCONDUCTIVITY,IOP TEAM — We report a detailed investigation on the lower critical field Hc1 of the superconducting Ba0.6K0.4Fe2As2 (FeAs-122) single crystals. A pronounced kink is observed on the Hc1(T) curve, which is attributed to the existence of two superconducting gaps. By fitting the data Hc1(T) to the two-gap BCS model in full temperature region, a small gap of Δa(0) = 2.0 ± 0.3 meV and a large gap of Δb(0) = 8.9 ± 0.4 meV are obtained. The in-plane penetration depth λab(0) is estimated to be 105 nm corresponding to a rather large superfluid density, which points to the breakdown of the Uemura plot in FeAs-122 superconductors.

1This work is supported by the Natural Science Foundation of China(973 project No: 2006CB60100, 2006CB921107, 2006CB921802), and Chinese Academy of Sciences (Project IITSNEM)
4:42PM T33.00012 Anisotropic London Penetration depth in NdFeAsO$_{0.9}$F$_{0.1}$ and Ba$_{0.55}$K$_{0.45}$Fe$_2$As$_2$ — CATALIN MARTIN, R.T. GORDON, M.A. TANATAR, H. KIM, M.E. TILLMAN, N. NI, P.C. CANFIELD, V.G. KOGAN, R. PROZOROV. Ames Laboratory and Department of Physics & Astronomy, Iowa State University, H. LOU, Z. WANG, H.H. WEN, National Laboratory for Superconductivity — In and out of plane London penetration depth was measured in single crystals of NdFeAsO$_{0.9}$F$_{0.1}$ (Nd-1111) and Ba$_{0.55}$K$_{0.45}$Fe$_2$As$_2$ (BaK-122) as a function of temperature by using an rf-resonator technique. In Nd-1111, penetration depth shows exponential behavior at low temperature, implying a fully-gapped Fermi surface. Superfluid density is best described in the full temperature range by a slightly anisotropic order parameter. In contrast, penetration depth of BaK-122 shows power-law temperature dependence ($\Delta \chi(T) \propto T^n$, $n \approx 2$) down to $T \approx 10$ K, and anisotropy $\gamma$ varies from 2 at $T_c$ to about 4 at 0.5 K. Possible symmetries of the gap consistent with such behavior and comparison with results from other techniques and with proposed theoretical models will be discussed. Also, the temperature dependence of the anisotropy $\gamma_{\Delta}(T)$ for both compounds, will be compared to that of $\gamma_{\Delta}(T)/\gamma_{\Delta}(0)$. In connection with possible multiband superconductivity.

4:54PM T33.00013 Muon Spin Relaxation Study of Ba(Fe$_{0.93}$Co$_{0.07}$)$_2$As$_2$ — GRAEME LUKE, A. ACZEL, McMaster University, J.P. CARLO, Columbia University, T. GOKO, TRIUMF, T.J. WILLIAMS, McMaster University, N. NI, S.L. BUD'KO, P.C. CANFIELD, Ames Laboratory, Y.J. UEMURA, Columbia University — We have performed muon spin relaxation ($\mu$SR) measurements of superconducting Ba(Fe$_{0.93}$Co$_{0.07}$)$_2$As$_2$. Zero field measurements show that static magnetism is absent for this Co concentration. In the mixed state, we observe a well-formed vortex lattice which results in an anisotropic $\mu$SR lineshape. We have fit the spectra to a microscopic model for the vortex state to obtain the magnetic field penetration depth. The penetration depth is about 2000Å in low (200G) fields and increases with applied field. The temperature dependence of the superfluid density is well described by a power law; behaviour which is consistent with gap nodes, substantial gap anisotropy or multi-band superconductivity. Research at McMaster University is supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

5:06PM T33.00014 Anisotropic superconducting properties of aligned Sm$_{0.95}$La$_{0.05}$FeAsO$_{0.85}$F$_{0.15}$ microcrystalline powder — H.C. KU, B.C. CHANG, C.H. HSU, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, Y.Y. HSU, Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan, Z. WEI, K.Q. RUAN, X.G. LI, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, China — The Sm$_{0.95}$La$_{0.05}$FeAsO$_{0.85}$F$_{0.15}$ compound is a quasi-2D layered superconductor with a superconducting transition temperature $T_c = 52$ K. Due to the Fe spin-orbital related anisotropic exchange coupling (antiferromagnetic or ferromagnetic fluctuation), the tetragonal microcrystalline powder can be aligned at room temperature using the field-rotation method where the tetragonal $ab$-plane is parallel to the aligned magnetic field $B_0$ and $c$-axis along the rotation axis. Anisotropic superconducting properties with anisotropic diamagnetic ratio $\chi_{\Delta}/\chi_{\Delta0} \approx 2.4 + 0.6$ was observed from low field susceptibility $\chi(T)$ and magnetization $M(B)$. The anisotropic low- field phase diagram with the variation of lower critical field gives a zero-temperature penetration depth $\lambda_0(0) = 280$ nm and $\lambda_{ab}(0) = 120$ nm. The magnetic fluctuation used for powder alignment at 300 K may be related with the pairing mechanism of superconductivity at lower temperature.

5:18PM T33.00015 Diminishing anisotropy of PrFeAsO$_{1-y}$ single crystal as temperature goes zero — DAICHI KUBOTA, TAKEKAZU ISHIDA, Osaka Pref Univ (Sakai), MOTOYUKI ISHIKADO, SHIN-ICHI SHAMOTO, JAEWON PARK, HIROSHI EISAKI, AIIST, HIJIRI KITO, AKIRA IYO, AIIST (Tsukuba) — The magnetic torque of a high-quality PrFeAsO$_{1-y}$ single crystal has been investigated at temperatures from 10 K to 45 K in magnetic fields from 5 KG and 50 KG. The torque curves of the PrFeAsO$_{1-y}$ single crystal have been measured systematically. The superconducting anisotropy of PrFeAsO$_{1-y}$ is determined by analyzing the torque curves. The temperature and field dependence of $\gamma$ reflect that the Fe-oxypnictide superconductivity has the rather three-dimensional isotropic nature of Fe-As layer network. We consider that this is good evidence for the multi-band superconductivity in Fe-oxypnictide. We find that the superconducting anisotropy $\gamma$ in PrFeAsO$_{1-y}$ can be approximated by $\gamma \approx 1.08 + 0.0068T$ in all fields by employing the Kogan model. We find it surprising to have such a low anisotropy parameter $\gamma$ even for a layered superconductor. Such a small anisotropic parameter in Fe-oxypnictides is preferential to ensure the intergrain connectivity and the resulting high critical current density $J_c$.

Wednesday, March 18, 2009 2:30PM - 5:30PM – Session T34 DCMP: Superconductivity: Vortex Statics and Dynamics 404

2:30PM T34.00001 Manipulation of interlayer "kinks" in individual vortices in underdoped YBa$_2$Cu$_3$O$_{6+x}$ — OPHIR AUSLAENDER, LAN LUAN, Stanford University, DOUGLAS BONN, RUIXING LIANG, WALTER HARDY, University of British Columbia, KATHRYN MOLER, Stanford University — We use magnetic force microscopy (MFM) to both image and manipulate individual vortex lines threading single crystalline YBa$_2$Cu$_3$O$_{6+x}$, a layered superconductor. We find that when we pull the top of a pinned vortex, it may not tilt smoothly, as in more isotropic superconductors [1]. In some cases, we observe a vortex breaking into discrete segments that can be described as short stacks of two-dimensional pancake vortices. This is similar to the "kinked" structure proposed by Benkraouda and Clem [2]. Quantitative analysis gives an estimate of the pinning force and the coupling between the pancake stacks. Our measurements highlight the discrete nature of stacks of pancake vortices in layered superconductors.


1 This work was partly supported by a Grant-in-Aid for Scientific Research from MEXT (Grant No. 19206104) and a special grant from Osaka Prefecture University.
2:42PM T34.00002 Moving flux quanta, driven by high density currents in low-impurity samples of V$_3$Si, LuNi$_2$B$_2$C, and NbSe$_2$: Ordered flow and core-size effects. S. MORAES, R.P. KHADKA, A.A. ČAPUD, U. of South Alabama; A.P. REYES, L.L. LUMATA, National High Magnetic Field Lab, J.R. THOMPSON, U. of Tennessee, D.K. CHRISTEN, Oak Ridge National Lab — There is incomplete understanding about the dissipative motion of magnetic flux quanta in type II superconductors, especially under large Lorentz forces. This is mainly due to the technical challenges involving the application of large electric currents and the rarity of samples wherein flux quanta are relatively free to move — i.e., samples with weak “pinning” — which commonly make it impossible to observe dynamic phases. Progress towards overcoming these challenges is described, along with clear observations of flux-flow phases in high-quality samples of three “low T$_c$” superconductors, V$_3$Si, LuNi$_2$B$_2$C, and NbSe$_2$. Evidence of the rarely observed Bardeen-Stephen flux flow — a highly ordered, collective motion of flux quanta in near-unison — will be presented. These observations have also enabled an examination of a model by Kogan and Zelezhina [Kogan and Zhelezina, Phys. Rev B 71, 134505 (2005)] predicting the effect of a field-dependent flux core size on ordered flux flow, as will be discussed. Funded by the U. of South Alabama and by the Research Corporation. We thank P. Canfield and L. Delong for samples and helpful discussions.

2:54PM T34.00003 Lattice slips in slow moving magnetic vortex lattices in NbSe$_2$. MICHAEL DREYER, JONGHEE LEE, HUI WANG, University of Maryland, BARRY BARKER, LPS — We studied vortex matter in NbSe$_2$, a type II superconductor, at magnetic fields of 0.25 - 0.75 T and temperatures of 4.2 K. At these fields the vortices form an Abrikosov lattice. Due to a small residual resistance in our superconducting magnet the applied magnetic field slowly decayed, driving the vortex lattice. The velocity was low enough to allow acquiring highly resolved time series using a low temperature scanning tunneling microscopy (STM). From the images we were able to extract local variations in the lattice constant as well as time series of the average vortex position (path) and velocity. A more subtle observation where closed loops on the order of nanometer in diameter in the averaged path of the vortices. Although this was observed in more than one data series it was at first dismissed as an artifact. Later, similar loops where observed in simulations. The loops occurred when a lattice dislocation traveled through the vortex lattice. This observation, unexpected in the simulation, gave new credence to the previously observed loops in the data. Since the vortex lattice in NbSe$_2$ was in the Bragg glass phase we would expect locally ordered domains of several micrometer in diameter. It is conceivable that lattice slips occur at the domain boundaries and lead to the observed loops. The observation and simulation will be compared in detail. We would like to thank Eva Andrej and Helmut Berger for providing NbSe$_2$ samples.

1This work was supported by the Laboratory for Physical Sciences

3:06PM T34.00004 Vortex interactions in superconducting weak-pinning channel ratchets$^1$, K. YU, T.W. HEITMANN, C. SONG, M.P. DEFEO, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — We report on measurements of vortex ratchets fabricated from weak-pinning superconducting a-NbGe channels bounded by strong-pinning NbN banks with asymmetric sawtooth edges. This configuration for the vortex confinement potential results in an asymmetric response for the vortex dynamics in the channels. Interactions between vortices, both within a channel and between neighboring channels, have a substantial influence on the ratchet behavior, including certain regimes where the net vortex motion through the ratchet reverses direction. We discuss our measurements in terms of a model for describing the vortex interactions in the ratchet channels.

$^1$Supported by NSF DMR-0547147

3:18PM T34.00005 Flux-flow noise in a superconducting Corbino vortex ratchet channel$^1$, T.W. HEITMANN, K. YU, C. SONG, M.P. DEFEO, B.L.T. PLOURDE, Syracuse University, M.B.S. HESSELBERTH, P.H. KES, Leiden University — We report measurements of vortex dynamics in a single nanofabricated weak-pinning vortex channel of a-NbGe with strong-pinning NbN channel edges. The channel is arranged in a circle on a Corbino disk geometry with a radial bias current, thus eliminating the influence of edge barriers to vortex entry on the dynamics and resulting in closed circular orbits for the vortices. An asymmetric sawtooth shape for the channel walls produces a ratchet effect, resulting in large differences in the critical current for the two flow directions. The SQUID picovoltmeter that we have developed for resolving the flux-flow voltage provides a low noise floor such that we can resolve structure in the flux-flow noise, with substantial asymmetries for vortex motion in the two directions through the ratchet channel.

$^1$Supported by NSF DMR-0547147


$^1$This work was supported by the FWO-Vl, the IAP, and the “Odysseus” program of the Flemish Government and FWO-Vl. V.R.M. is funded by the EU Marie Curie project, Contract No. MIF1-CT-2006-040816.

3:42PM T34.00007 Vortex dynamics simulation in high-$T_c$ superconductors with planar pinning arrays coexisting with point pinning sites. HIDEHIRO ASAI, SATOSHI WATANABE, University of Tokyo — The enhancement of critical currents $I_v$ by introducing artificial pinning sites is key issue in the application of high-$T_c$ superconductors. Planar defects such as twin boundary are well known as the possible candidates for tangible pinning sites. Recently, the improvement of $I_v$ has been reported in the samples having high-density planar defects. However, the pinning characteristics of planar defects, especially the change of the pinning efficiency in the presence of point pinning, are still unclear. We have studied the dynamics of vortices interacting with both planar pinning and point pinning sites using molecular dynamics simulation. We have fixed the pinning strength of planar pinning, and calculated the $I_v$ as a function of the point pinning strength $J_p$. With increasing $J_p$, $I_v$ changes from $I_v = I_{p0}$ ($J_p$: $I_v$ obtained in the system without point pinning) to $I_v = I_{p0} + \alpha$ ($J_p$: $I_v$ obtained in the system without planar pinning) and then to $I_v = J_p$. This behavior corresponds to the appearance of the kink structure and the drastic change of c-axis correlation function of the vortices. We have also performed the similar calculation with different anisotropy parameters and observed that the stiffness of vortex line changes the $I_v$ behavior as a function of $J_p$.
3:54PM T34.00008 The Peak Effect anomaly in low and high Tc superconductors: stable and metaestables vortex lattice configurations, VICTORIA BEKERIS, GABRIELA PASQUINI, DIEGO PEREZ DAROCA, CLAUDIO CHILOTTE, GUSTAVO LOZANO, Departamento de Fisica, FCEyN, Universidad de Buenos Aires, Pabellon I Ciudad Universitaria, Buenos Aires, Argentina. — Competing interactions in the vortex lattice (VL) of type II superconductors give rise to an order-disorder transition known as Peak Effect (PE) anomaly. The strong metaestability related to the PE masks the stationary VL configurations (VLCs), both in low and in high Tc superconductors. By means of linear ac susceptibility experiments, that avoid VL reorganization, we explore quasi-static stable and metastable states, applying different shaking protocols before measurements. In low Tc NbxSe2 crystals we identify TH regions where stationary configurations are maximally ordered (Bragg Glass), fully disordered or where ordered and disordered stable phases coexist. In contrast, in high Tc Yb2As3 (G07) crystals, metaestability seems to dominate and different metastable VLCs are accessed depending on the previous dynamic history, with no access to the lowest energy configuration. [1] G. Pasquini et al. Phys. Rev. Lett. 100, 247003 (2008)

4:06PM T34.00009 Dynamics of Josephson vortices mediated with pancake vortices, KAZUTO HIRATA, National Institute for Materials Science, SHUUICHI OOI, TAKASHI MOCHIKU, PHYSICAL PROPERTIES TEAM — Josephson vortices (JVs) flow very fast with a velocity up to tenth of the light velocity in Bi-2212. If the motion of JVs can be controlled, high-speed signal processing will be achieved. We have tried to apply symmetrical pinning centers in space and time-asymmetric input signals for controlling a dynamical behavior of JVs in Bi-2212. We have shown the periodic oscillations in JV flow-resistance against magnetic field in Bi-2212 (PRL99(2002)247002), which persist in wide range of temperature and magnetic field. Introducing pancake vortices (PVs) into JV system in Bi-2212, the JV flow-resistance abruptly decreases, because the JVs interact with the PVs strongly and the PVs are pinned in intrinsically existing pinning centers in Bi-2212. However, when the input current (signal) with two frequencies is applied, a finite dc voltage can be obtained even without the flow-resistance. This leads to a rectification effect in the JVs’ motion by the PVs. The nonlinearity in I-V characteristics induces the rectification effect with time-asymmetric input signals of two harmonics. This may open a new application of HTSCs.

4:18PM T34.00010 Exploring the Aging Effects in Pinned Vortex Lattices in Nb using Neutron Reflectometry, XI WANG, HELEN HANSON, XINSHENG LING, Brown University, BRIAN MARANVILLE, NIST — We report the first experiment using neutron reflectometry to explore the aging effects in pinned vortex lattices in Nb. A striking prediction of the Bragg glass model is the existence of a pinned elastic Bragg glass solid matter in the vortex state of weakly disordered type-II superconductors. According to this model, the system is pinned in the random-manifold regime with local metastable states, yet at large length scale, the system remains elastic. This seemingly paradoxical property is predicted to lead to novel aging dynamics. This work was supported by a grant from DOE-BES. The experiments were carried out at NG-1- Advanced Neutron Diffraction facility at NIST NCNR.

4:30PM T34.00011 Measurement of Vortex Bragg Glass Structure Factor in Nb using Neutron Reflectometry, HELEN HANSON, XI WANG, XINSHENG LING, Brown University, BRIAN MARANVILLE, NIST — One of the key predictions in the Bragg Glass model of weakly pinned vortex lattices is a power-law structure factor similar to that of a 2D solid. Previous attempts using SANS in Nb and HTSC have provided results that are consistent with the Bragg model. Here we report the first experiment using neutron reflectometry to resolve S(Q) in a Nb single crystal. This work was supported by a grant from DOE-BES. The experiments were carried out at NG-1- Advanced Neutron Diffraction facility at NIST NCNR.

4:42PM T34.00012 Small-angle neutron scattering study of vortex matter in superconducting Ba(Fe0.93Co0.07)2As2, M. R. ESKILDSEN, University of Notre Dame, T. BLASIUS, University of Michigan, A. I. GOLDMAN, Ames Laboratory and Iowa State University, J. M. DENSMORE, University of Notre Dame, C. D. DEWHURST, Institut Laue-Langevin, N. NI, A. KREYSSIG, S. L. BUD’KO, P. C. CANFIELD, Ames Laboratory and Iowa State University — We present small-angle neutron scattering studies of the superconducting vortices Ba(Fe0.93Co0.07)2As2. At all fields measured a ring of scattering was observed, indicating a highly disordered vortex configuration, and no discernable rocking curve could be measured. The field dependence of the magnitude of the scattering vector indicates vortex lattice domains of (distorted) hexagonal symmetry. An analysis of the scattered intensity due to the vortices shows a rapid decrease with increasing applied magnetic field, significantly exceeding what would be expected based on estimates of the upper critical field. These results are consistent with the existence of a vortex glass or Bragg glass phase in Ba(Fe0.93Co0.07)2As2.

1Supported by NSF through grant DMR-0804887. Work at Ames Lab is supported by the U. S. DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

4:54PM T34.00013 Pauli Paramagnetic Effects in the Mixed State of CeCoIn5 Revealed by Small Angle Neutron Scattering, P. DAS, M. R. ESKILDSEN, L. DEBEER-SCHMITT, University of Notre Dame, IN, USA, J. S. WHITE, E. M. FORGAN, University of Birmingham, UK, A. D. BIANCHI, Universite de Montreil, Canada, M. KENZELMANN, J. L. GAVILANO, M. ZOLLIKER, S. GERBER, J. MESOT, ETHZ & Paul Scherrer Institute, Switzerland, C. WANG, E. D. BAUER, J. L. SARRAO, Los Alamos National Lab, NM, USA, C. PETROVIC, Brookhaven National Lab, NY, USA. — We report on extensive small-angle neutron scattering measurements on the vortex lattice (VL) in the mixed state of CeCoIn5, with the magnetic field (H) both parallel and perpendicular to the c-axis. We obtain the H- and T-dependence of the form factor (|F|2) - a measure of the field contrast in the mixed state. At low T, competition between Pauli paramagnetism and the antiparallel spin alignment of f-wave pairing gives “magnetized” VL cores, causing |F|2 to increase with H [1]. We observe a crossover to a state where |F|2 falls again near Hc2, the falling off extends outside the proposed FFLO region and is believed to arise from expansion of the magnetized cores. This core expansion may also explain the sequence of VL phase transitions observed in this material. At higher T, we observe a crossover towards more conventional behavior.

5:06PM T34.00014 Vortex phase diagram in weakly pinned Rh17S15, S. RAMAKRISHNAN, H. R. NAREN, ARUMUGAM TAMIZHAVEL, ARUN GROVER, TIFFR. — A vortex phase diagram of the strongly correlated superconductor Rh17S15 has been constructed via exploration of the anomalous variations in critical current density extracted from ac and dc magnetization measurements. The iso-field in-phase susceptibility experiments, that avoid VL reorganization, we explore quasi-static stable and metastable states, applying different shaking protocols before measurements. In low Tc NbxSe2 crystals we identify TH regions where stationary configurations are maximally ordered (Bragg Glass), fully disordered or where ordered and disordered stable phases coexist. In contrast, in high Tc Yb2As3 (G07) crystals, metaestability seems to dominate and different metastable VLCs are accessed depending on the previous dynamic history, with no access to the lowest energy configuration. [1] G. Pasquini et al. Phys. Rev. Lett. 100, 247003 (2008).

5:18PM T34.00015 ABSTRACT WITHDRAWN
2:30PM T35.00001 Role of fluorine in the iron pnictides: phonon softening and effective hole-doping¹, JESSE NOFFSINGER, FELICIANO GIUSTINO², STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — Using first principles techniques, we investigate the influence of fluorine doping on the electronic structure, lattice dynamics and electron-phonon coupling in LaFeAsO. We explicitly simulate the F-doping using a supercell model in order to explore properties not described by virtual crystal models. Our analysis reveals that local lattice relaxation accompanies the fluorine doping and modifies the lattice dynamics, in accord with recent experimental data. In addition, it is found that the charge density of the doped electrons cannot be described by simplified models of electron-doping in the two-dimensional Fe-plane.

¹This work was supported by National Science Foundation Grant No. DMR07-05941, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory’s NERSC facility.

²Present Address: Dept. of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK

2:42PM T35.00002 Effects of Magnetic Ordering on Phonon Spectra in Iron-based Superconductors: First Principle Calculation and Theoretical Analysis¹, HIROKI NAKAMURA, MASAHIKO MACHIDA, CCSE, JAEA, ALFRED BARON², Spring-8/RIKEN, TATSUO FUKUDA³, Spring-8/JAEA, SHINICHI SHAMOTO⁴, MNRC JAEA — Recently, inelastic x-ray scattering measurements on single crystals of PrFeAsO₁₋₀.₂ have reported that phonons related with Fe-Fe and Fe-As bondsings are significantly more softened than those obtained by the first principle calculations [1]. However, it is noted that any previous calculations do not include the magnetic degree of freedom. Therefore, we performed the phonon structure calculations by taking into account the magnetic structure in mother compounds. The magnetic calculations are in better agreement with the observed softening. We show the results and clarify the reason.

¹JSPS, Superclean MEXT Project
²CREST JST & TRIP JST
³CREST JST & TRIP JST
⁴TRIP JST
⁵TRIP JST
⁶TRIP JST

2:54PM T35.00003 Cubic anharmonicity of the Fe-As bond of the iron-pnictides estimated from Raman spectroscopy. MATS GRANATH, Gothenburg University, JOHAN BIELECKI, JOAKIM HOLMLUND, CHRIS KNEE, Chalmers University of Technology, NAN LIN WANG, Beijing National Laboratory for Condensed Matter Physics, LARS BÖRJESSON, Chalmers University of Technology — We study the phonon spectrum of the iron-pnictide superconductors, (Ce,Nd)O₁₋₀.₃₅FeAs, using Raman spectroscopy. Based on the temperature dependent softening of the out of plane optical Fe-mode (B₁g, at 1') we estimate the magnitude of the cubic anharmonicity of the Fe-As bond by calculating the self-energy due to phonon-phonon interactions. This also gives an estimate of the lattice expansion or contraction due to Fe isotope substitution which may in turn influence electronic properties.

3:06PM T35.00004 Phonon Softening in PrFeAsO₁₋₀.₂ by Inelastic X-Ray Scattering¹, ALFRED Q.R. BARON, SPRING8/RIKEN and JASRI, TATSUO FUKUDA, SPRING8/RIKEN and JAEA, SHIN-ICHI SHAMOTO, JAEA, HIROSHI UCHIYAMA, SPRING8/JASRI, JUN-ICHIRO MIZUKI, JAEA, HIROKI NAKAMURA, MASAHIKO MACHIDA, CREST, JST, JAEA, MOTOYUKI ISHIKADO, JAEA, MASATOSHI ARAI, J-PARC JAEA, HIJIRI KITO, HIROSHI EISAKI, NERI, AIST — We present phonon dispersion measurements from single crystals of PrFeAsO₁₋₀.₂ with Tₐ (onset) of 42 to 45 K made using inelastic x-ray scattering with 1.5 meV resolution at BL35XU of SPring-8. In agreement with our previous results on powders and crystals [1] we see pronounced softening of the in-plane Fe-As modes compared to phonon calculations using pseudopotential methods in the tetragonal (non-magnetic) structure. C-axis modes are somewhat harder. No strong changes in phonon spectra across Tₐ were observed at the momentum transfers investigated. We also compare our results against calculations of phonons in the magnetic parent material. [1] Fukuda, et al., J. Phys. Soc. Japan, 77 (2008), 103715.

¹Support by the JST program for Transformative Research-Project on Iron Pnictides (TRIP) is gratefully acknowledged

3:18PM T35.00005 CaFe₂As₂ Phonons via Inelastic X-ray Scattering and First Principles Calculations, STEVEN HAHN, Ames Laboratory and Iowa State University, AHMET ALATAS, BOGDAN LEU, Advanced Photon Source, Argonne National Laboratory, YONGBIN LEE, NI, Ames Laboratory and Iowa State University, DUCK YOUNG CHUNG, ILIYA TODOROV, Materials Science Division, Argonne National Laboratory, MERCOURI KANTZIDIS, Materials Science Division, Argonne National Laboratory and Department of Chemistry, Northwestern University, ERCAN ALP, Advanced Photon Source, Argonne National Laboratory, PAUL CANFIELD, ALAN GOLDMAN, ROBERT MCQUEENFY, BRUCE HARMON, Ames Laboratory and Iowa State University — In the iron pnictides, the sensitivity of the iron magnetic moment to the arsenic position suggests a strong relationship between phonons and magnetism. We measured the phonon dispersion of several branches in the high temperature tetragonal phase of CaFe₂As₂ using inelastic x-ray scattering on single-crystal samples. These measurements were compared to ab-initio calculations of the phonons. Spin polarized calculations imposing the antiferromagnetic order present in the low temperature orthorhombic phase dramatically improves agreement between theory and experiment. This is discussed in terms of the strong antiferromagnetic correlations that are known to persist in the tetragonal phase.

3:30PM T35.00006 Magnetic and lattice coupling in the AFe₂As₂ (A=Ca, Ba, and Sr) compounds¹, HAIFENG LI, DAVID VAKNIN, JEREL ZARESTKY, WEI TIAN, ANDREAS KREYSSIG, NI NI, SERGEY BU’DKO, PAUL CANFIELD, ROBERT MCQUEENFY, ALAN GOLDMAN, Ames Laboratory and Physics Department and Astronomy, Iowa State University, Ames, IA — Systematic elastic and inelastic neutron scattering studies of the AFe₂As₂ (A=Ca, Ba, and Sr) compounds reveal some common and distinguished properties that may shed light on the nature of the coupling between the magnetic and lattice degrees of freedom. We find, that for all three samples, the structural and antiferromagnetic (AFM) transition temperatures coincide within the experimental uncertainty of measurements. We also find that the AFM propagation vector is unequivocally along the long a- orthorhombic axis for all three compounds. The coupling between the magnetic and chemical structure is in play below the transition down to the lowest temperatures. More results and discussion on the nature of the transitions will be presented.

¹Supported by the U.S. DOE under Contract No. DE-AC02-07CH11358.
3:42PM T35.00007 Large electron-A_{1g} phonon interaction in doped LaOFeAs: coupling with antiferromagnetism1, FELIX YNDRUAIR, JOSE SOLER, Universidad Autonoma de Madrid — We present first principles calculations of the atomic and the electronic structure of electron-doped LaOFeAs. We find that whereas the undoped compound has an antiferromagnetic arrangement of magnetic moments at the Fe atoms, the doped system becomes non magnetic at a critical electron concentration. We have studied the electron-phonon interaction in the doped paramagnetic phase. For the A_{1g} phonon, the separation between the As and Fe planes induces a non-collinear arrangement of the Fe magnetic moments. This arrangement is anti parallel for interactions mediated by As, and perpendicular for Fe-Fe direct interactions, thus avoiding frustration. This coupling of magnetism with vibrations induces anharmonicities and an electron-phonon interaction much larger than in the pure paramagnetic case. We propose that such enhanced interactions play an essential role in superconducting compounds close to an antiferromagnetic phase transition.

1Supported by the Spanish Ministry of Science and Innovation through grants FIS2006-12117 and CSD2007-00050.

3:54PM T35.00008 Phonon and magnetic excitations in the novel BaFe1.8Co0.2As2 superconductor, DAN PARSHALL, Univ of Tennessee, Dept of Physics, KONSTANTIN LOKSHIN, Univ of Tennessee, Dept of Materials Science, MATTHEW STONE, DOUGLAS ABERNATHY, MARK LUMSDEN, ANDREW CHRISTIANSON, DAVID MANDRUS, ATHENA SAFAF-SEFAT, ORNL, TAKESHI EGAMI1, ORNL, Univ of Tennessee, Dept of Physics and Materials Science — Phonon and magnetic excitations in the BaFe1.8Co0.2As2 superconductor single crystal were studied by inelastic neutron scattering using the ARCS time-of-flight spectrometer at the Spallation Neutron Source. Most of the phonon branches show a good agreement with the density functional theory calculations. However, the As-Raman vibrations along the c-axis demonstrate strong softening contrary to the flat behavior expected from the LDA calculations. The softening is strongest along the (0.5, 0.5, L) direction by up to 4 meV. At the same time a sharp magnetic response was found along the same (0.5, 0.5, L) direction over a wide range of L-values at energy transfer of 10-25 meV. This dynamic magnetic responses indicates on a 2-D character of antiferromagnetic spin fluctuations in the superconducting phase, in strong contrast to the 3-D static antiferromagnetism in the undoped non-superconducting BaFe2As2. Thus, in Fe-As based superconductors magnetism shows strong sensitivity to the lattice, suggesting a possibility of spin-phonon coupling playing a role in superconductivity.

1corresponding author

4:06PM T35.00009 3d crystal field excitations in iron pnictides studied by Raman spectroscopy, TAO ZHOU, ZHEN QIN, SEAN O’MALLEY, KWOK LO, New Jersey Institute of Technology, CHENG LIN ZHANG, SANG-WOOK CHEONG, Rutgers University — We have measured the Raman spectra of LaFeAsO1-xFx (x = 0, 0.1 and 0.33) as well as A2Fe2As2 (A = Ca, Sr, Ba) polycrystalline samples at different temperatures. We found that in addition to the phonon excitations at low frequency below 250 cm\(^{-1}\), there are many strong excitations in the range between 250 cm\(^{-1}\) and 1000 cm\(^{-1}\). We attribute them to the crystal field excitations of Fe 3d electrons. This down turn in the Cp/T vs. T\(^2\) plot, however, is suppressed in both poly-crystal samples and under high fields. We attribute this feature to the crystal field excitations of Fe 3d electrons.

4:18PM T35.00010 Evidence for two gaps from specific heat in LiFeAs single crystals, FENGYAN WEI, Texas Center for Superconductivity at University of Houston and Department of Physics, BING LV, Texas Center for Superconductivity at University of Houston and Department of Physics — We have measured the Raman spectra of LaFeAsO1-xFx (x = 0, 0.1 and 0.33) as well as A2Fe2As2 (A = Ca, Sr, Ba) polycrystalline samples at different temperatures. We found that in addition to the phonon excitations at low frequency below 250 cm\(^{-1}\), there are many strong excitations in the range between 250 cm\(^{-1}\) and 1000 cm\(^{-1}\). We attribute them to the crystal field excitations of Fe 3d electrons. This down turn in the Cp/T vs. T\(^2\) plot, however, is suppressed in both poly-crystal samples and under high fields. We attribute this feature to the crystal field excitations of Fe 3d electrons.

4:30PM T35.00011 Coexistence of superconductivity and ferromagnetism in BaFe1.8Co0.2As2, MARIO S. DA LUZ, Montana State University, R. K. BOLLINGER, Montana State University, J. J. NEUMEIER, Montana State University, A. SEFAT, M. A. MCGUIRE, R. JIN, B. C. SALES, M. MANDRUS, Oak Ridge National Laboratory — Thermal expansion and heat capacity measurements were performed on three single crystals of BaFe1.8Co0.2As2 with superconducting transition temperatures \(T_c = 16.5, 19, \) and 22 K. The thermal expansion coefficients \(\gamma_i\) (i = a, b, c) were determined. Magnetization measurements reveal the presence of ferromagnetism at the same temperature transition as superconductivity in some of the samples. The ferromagnetism has a small moment on the order of 0.5x10\(^{-3}\) \(\mu_B/\text{Fe (Bohr magneton)}\). Thus, two phases: superconductivity and magnetism coexist in some BaFe1.8Co0.2As2 samples. This ferromagnetism could be associated with a canted (non- collinear) antiferromagnetic order. This material is based upon work supported by the U. S. Department of Energy (DE-FG02-07ER46259) and the National Science Foundation (DMR-050476 and DMR-052458).

4:42PM T35.00012 Comprehensive Characterization of Superconductivity in Co-doped BaFe2As2, TSUYOSHI TAMEGAI, YASUYUKI NAKAJIMA, TOSHIHIRO TAEN, Dep. of Appl. Physics, The University of Tokyo — We have grown high-quality single crystals of BaFe2As2 by self-flux method. Superconducting properties of these single crystals are characterized by measuring magnetization, resistivity, upper critical field, Hall coefficient, and magneto-optical images. A sharp drop of susceptibility is observed around 24 K for x=0.1. Irreversible magnetization shows fish-tail feature in a wide temperature range, indicating the presence of inhomogeneities in the crystal. The critical current density \(J_c\) for \(x=0.1\) is over \(10^6\) A/cm\(^2\) at low temperatures up to 50 K. Upper critical field determined by resistive transition is anisotropic with anisotropic \(J_c\). Hall effect measurements indicate that \(BaFe_{1-x}Co_xAs_2\) is a multiband system with a dominant conduction by electron. Magneto-optical image for \(x=0.1\) at 25 K reveals the presence of trapped vortices in a part of the crystal, which leads us to expect that bulk superconductivity above 25 K can be realized by fine tuning the Co-doping level.

1This work is partly supported by JST, Transformative Research-Project on Iron Pnictides (TRIP)

4:54PM T35.00013 Superconductivity in Sr(Fe,Ni)2As2 single crystals, NICHOLAS BUTCH, SHANTA SAHA, KEVIN KIRSHENBAUM, JOHNPIERRE PAGLIONE, Center for Nanophysics and Advanced Materials, Dept. of Physics, University of Maryland, College Park — Iron pnictide compounds are the subject of intense research efforts because of their relatively high superconducting critical temperatures and the interplay of magnetic, structural, and superconducting phases found in these materials. Of the known superconducting iron pnictide compounds, those with the ThCr2Si2 structure appear to have the best chemical homogeneity. We present transport, magnetic, and specific heat measurements of Ni-substituted SrFe2As2 flux-grown single crystals.

1NBP is supported by the CNAM Glover Postdoctoral Fellowship.
In the established LDA+ experimental values. The implementation within the KKR band structure method. density approximation method, implemented within multiple scattering theory. We briefly describe the formalism and discuss important technical issues of its

Laboratory, UK — In this work we study the electronic structure of 3d-transition metal oxides as obtained with the self-interaction corrected-local spin f positions of the occupied and unoccupied localized UC Sant Barbara, CA 93106 — Understanding the physics of f systems, characterized by the competition between itinerant (delocalized) and highly localized f-states, is regarded as a great challenge in condensed-matter physics today. As a first step towards a systematic ab initio understanding of f-electron systems, we apply many-body perturbation theory in the $G_0W_0$ approach based on LDA+$U$ ground state calculations ($G_0W_0$) to a selected set of lanthanide oxides (CeO$_2$ and Ln$_2$O$_3$ (Ln=lanthanide series)). These compounds have important technological applications, in particular in catalysis and microelectronics. We demonstrate good agreement between the $G_0W_0$ density of states (DOS) and experimental spectra for CeO$_2$ and Ce$_2$O$_3$. For the whole Ln$_2$O$_3$ series $G_0W_0$ reproduces all main features found for the optical experimental band gaps. Inspection of the DOS reveals that the relative positions of the occupied and unoccupied f-states predicted by $G_0W_0$ confirm the experimental conjecture derived from phenomenological arguments.

2:30PM T36.00001 New approach on calculating Green’s functions in Full-Potential Multiple Scattering Methods. AURELIAN RUSANU, Oak Ridge National Laboratory, YANG WANG, Pittsburgh Supercomputing Center, G. M. STOCKS, Oak Ridge National Laboratory, JOHN S. FAULKNER, Florida Atlantic University — The most common methods of computing Green’s functions in modern full-potential multiple scattering applications rely on solving Schrödinger (Dirac) equations for regular and irregular solutions of a single-site scatterer over an energy contour in the complex plane. While, for spherical potentials, the standard formulae for calculating the Green’s function are numerically stable they often result in unphysical behavior for non-spherical potentials, particularly close to the nucleus and for large angular momentum quantum numbers. Here we use a new analytical and numerical method that does not require calculation of the irregular solution, to which the numerical instability can be traced. The new approach results in the correct analytic behavior and numerical stability.

1Research sponsored by the Division of Materials Science and Engineering, U.S. DOE, Oak Ridge National Laboratory with UT-Battelle, LLC.

2:42PM T36.00002 Local excitations in charge-transfer insulators: a super atom approach via Wannier functions CHI-CHENG LEE, WEIGUO YIN, Brookhaven National Laboratory, WEI KU, Brookhaven National Laboratory and SUNY Stony Brook University — Local excitations in strongly correlated charge-transfer insulator are very often tied to the rich functionalities of these materials. However, these tightly bound local excitations prove to be difficult to calculate from first-principles. In particular, the strong local interactions render the typical first-principles perturbation approach (via diagrammatic Bethe-Salpeter equation) inapplicable to describe the multiplets. In this talk, our recent progress in evaluating the local excitations in NIO will be presented. Utilizing the gauge freedom of the Wannier functions, the oxygen (charge-transfer) degrees of freedom can be integrated into a “super atom”, in which the strong local interactions can be incorporated on the equal footing as the strong coupling between the oxygen p- and Ni d- orbitals. Our results lead to good agreement with recent non-resonant inelastic X-ray scattering data [1] and the cluster calculation [2] for both q-dependence and excitation energies. Finally, extension to propagation of the local excitation will be addressed to include the dispersion in momentum space.

1Supported by the DOE and the Division of Scientific User Facilities U.S. DOE.

2:54PM T36.00003 Self-healing diffusion quantum Monte Carlo algorithms: Theory and Applications F.A. REBOREDO, P.R.C. KENT, M.L. TIAGO, Oak Ridge National Laboratory, R.Q. HOOD, Lawrence Livermore National Laboratory — We present a method to obtain the fixed node ground state wave function from an importance sampling Diffusion Monte Carlo (DMC) run. The fixed node ground state wave-function is altered to obtain an improved trial wave-function for the next DMC run. The theory behind this approach will be discussed. Two iterative algorithms are presented and validated in a model system by direct comparison with full configuration interaction (CI) wave functions and energies. We find that the trial wave-function is systematically improved. The scalar product of the trial wave-function with the CI result converges to 1 even starting from wave-functions orthogonal to the CI ground state. Similarly, the DMC total energy and density converges to the CI result. In the optimization process we find an optimal non-interacting nodal potential of density-functional-like form. An extension to a model system with full Coulomb interactions demonstrates that we can obtain the exact Kohn-Sham effective potential from the DMC data. Subsequently we apply our method to real molecules such as benzene and find that we can improve the ground state energy as compared with the single determinant result even starting from random wave-functions. Results for other molecular systems and comparison with alternative methods will be presented.

3:06PM T36.00004 Removal of residual nonspherical self-interaction error in LDA+$U$ FEI ZHOU, VIDVUDS OZOLINS, UCLAn — In the established LDA+$U$ method, the electron self-interaction, which is generally nonspherical and orbital-dependent, is removed in a mean-field way. This results in residual self-interaction errors, particularly pronounced for f-electrons. An alternative double counting scheme that modifies the exchange, not Hartree, energy of LDA is proposed as a remedy. We show that LDA+$U$ with our approach preserves the expected degeneracy of f$^1$ and f$^2$ states in free ions and the correct ground states in the PrO$_2$ solid.

3:18PM T36.00005 The f-electron challenge: localized and itinerant states in lanthanide oxides united by GW@LDA+$U$ MATTHIAS SCHEFFLER, HONG JIANG, RICARDO I. GOMEZ-ABAL, FHI, Berlin, Germany, PATRICK RINKE, UC San Barbara, CA 93106 — Understanding the physics of f-electron systems, characterized by the competition between itinerant (delocalized) and highly localized f-states, is regarded as a great challenge in condensed-matter physics today. As a first step towards a systematic ab initio understanding of f-electron systems, we apply many-body perturbation theory in the $G_0W_0$ approach based on LDA+$U$ ground state calculations ($G_0W_0$) to a selected set of lanthanide oxides (CeO$_2$ and Ln$_2$O$_3$ (Ln=lanthanide series)). These compounds have important technological applications, in particular in catalysis and microelectronics. We demonstrate good agreement between the $G_0W_0$ density of states (DOS) and experimental spectra for CeO$_2$ and Ce$_2$O$_3$. For the whole Ln$_2$O$_3$ series $G_0W_0$ reproduces all main features found for the optical experimental band gaps. Inspection of the DOS reveals that the relative positions of the occupied and unoccupied f-states predicted by $G_0W_0$ confirm the experimental conjecture derived from phenomenological arguments.

3:30PM T36.00006 Self-interaction correction in multiple scattering theory — Application to transition metal oxide MARKUS DAENE, Oak Ridge National Lab, WOLFRAM HERGERT, Martin Luther University Halle, Germany, ARTHUR ERNST, Max Planck Institute for Microstructure Physics, Halle, Germany, MARTIN LUEDERS, ZDZISLAW SZOTEK, WALTER TEMMERMAN, Daresbury Laboratory, UK — In this work we study the electronic structure of 3d-transition metal oxides as obtained with the self-interaction corrected-local spin density approximation method, implemented within multiple scattering theory. We briefly describe the formalism and discuss important technical issues of its implementation within the KKR band structure method. We present results of such important properties as lattice constants, local magnetic moments, band gaps and discuss them in comparison with the LSD and the experimental values.
3:42PM T36.00007 Computational Modeling of Actinide Complexes Pertinent to Environment — KRISHNAN BALASUBRAMANIAN, Lawrence Livermore National Lab — We discuss computational projects relevant to actinide separation, complexes and the possibility of actinide sequestration by engineered mesoporous materials. We have carried out computational studies on a number of actinide complexes in aqueous solution; as such complexes are of considerable importance in our understanding of behavior of actinide species in the environment and high level nuclear waste, especially experimental-theoretical collaboration on curium (III) complexes with multi-dentate ligands with Nitsche and coworkers at LBLNL. Cu(III) complexes with phosphonic acid (PFA) were studied for assessing relative binding strengths of the two ligands with varying pH. Possible isomers of CmH2PPA2+ and CmHPPA+ 13C NMR spectra and bond geometry will be discussed. The effects of the aqueous solvent in the configuration preferences of CmH2PPA2+ and We have also studied aqueous complexes of U(VI), Np(VI) and Pu(VI) with OH-. We will discuss the results of our extensive ab initio computations on the equilibrium structure, infrared spectra, and bonding characteristics of a variety of hydrated NpO2(CO3)3^2- complexes by considering the solvent as a polarizable dielectric continuum as well as the corresponding anhydrate complexes in the gas-phase. The work at CSU Eastbay was supported in part by Office of Basic Energy Sciences of DOE, and the work at LLNL was carried out under contract number W-7405-Eng-48.

3:54PM T36.00008 The converse approach to NMR chemical shifts from first-principles: application to finite and infinite aromatic compounds — T. THONHAUSER, Wake Forest University, D. CERESOLI, N. MARZARI, MIT — We present first-principles, density-functional theory calculations of the NMR chemical shifts for polycyclic aromatic hydrocarbons, starting with benzene and increasing sizes up to the one- and two-dimensional infinite limits of graphenic ribbons and graphene. These calculations are performed using a combination of the recently developed theory of orbital magnetization in solids, and a novel approach to NMR calculations where chemical shifts are obtained from the derivative of the orbital magnetization with respect to a microscopic, localized magnetic dipole. Using these methods we study on equal footing the 1H and 13C shifts in benzene, pyrene, coronene, in naphthalene, anthracene, naphthacene, and pentacene, and finally in graphene, graphite, and an infinite graphene ribbon. Our results show very good agreement with experiments and allow us to characterize the trends for the chemical shifts as a function of system size.

4:06PM T36.00009 NMR chemical shifts from first-principles using the converse approach in periodic boundary conditions — DAVIDE CERESOLI, TIMO THONHAUSER, MIT, NICOLA MARZARI — An alternative, converse approach to the first-principles calculation of NMR shielding tensors can be formulated where NMR chemical shift are obtained from the derivative of the orbital magnetization with respect to the application of a microscopic, localized magnetic dipole. We apply here the modern theory of orbital magnetization to validate this formalism to the case of extended systems in periodic boundary conditions, finding very good agreement with established methods and experimental results. These results underscore the advantages of the converse approach over existing methods: (1) it can be applied to either isolated or periodic systems, (2) it avoids any linear response calculation, allowing to treat systems containing hundreds of atoms, and (3) it is not plagued by the gauge-origin problem.

4:18PM T36.00010 MP2 and RPA applied to solid state systems 1 — MARTIJN MARSMAN, Faculty of Physics, University Vienna, ANDREAS GRUENEIS, JUDITH HARL, GEORG KRESSE — We present ab initio total energy calculations at the level of Hartree-Fock + 2nd-order Møller-Plesset perturbation theory (HF+MP2), and the random-phase-approach within the framework of the adiabatic-fluctuation-dissipation-theorem (ACFDT-RPA), for extended systems under periodic boundary conditions, using plane wave basis sets. We characterize and compare the accuracy of these methods with respect to their description of the lattice constants, bulk moduli, and atomizations energies of several archetypical solid state systems. Furthermore, we present calculations of HF+MP2 quasiparticle gaps and compare them to results obtained within the GW approximation to the electronic self-energy.

4:30PM T36.00011 Bridging the size gap between density-functional and many-body perturbation theory — PAOLO UMARI, CNR-INFM Dimocritos — The calculation of quasi-particle spectra based on the GW approximation is extended to systems of hundreds of atoms and the calculation of empty states is avoided. This is achieved through an optimal strategy, based on the use of Wannier-like orbitals, for obtaining a basis for the polarization propagator. Then, a Lanczos chain approach permits to calculate the self-energy. Our method is validated by calculating the vertical ionization energies of the benzene molecule and the band structure of crystalline silicon. Its potentials are then demonstrated by addressing the quasi-particle spectrum of models of vitreous materials, as well as of large organic molecules.

4:42PM T36.00012 Quasiparticle properties of DNA bases from GW calculations in a Wannier basis — XIAOFENG QIAN, NICOLA MARZARI, Department of Materials Science and Engineering, MIT, PAOLO UMARI, Theory at Elettra Group, CNR-INFM Dimocritos, Basovizza (Trieste), Italy — The quasiparticle GW-Wannier (GWW) approach [1] has been recently developed to overcome the size limitations of conventional GW and wave function calculations. By taking advantage of the localized properties of the maximally-localized Wannier functions and choosing a small set of polarization basis we reduce the number of Bloch wavefunctions products required for the evaluation of dynamical polarizabilities, and in turn greatly reduce memory requirements and computational efficiency. We apply GWW to study quasiparticle properties of different DNA bases and base-pairs, and solvation effects on the energy gap, demonstrating in the process the key advantages of this approach. [1] Umari, G. Stenuit, and S. Baroni, cond-mat/0811.1453

5:06PM T36.00013 Reliable Prediction of Charge Transfer Excitations in Molecular Complexes — LEEOR KRONIK, Weizmann Institute of Science, Israel, TAMAR STEIN, ROI BAER, Hebrew University of Jerusalem, Israel — We show how charge transfer excitations at molecular complexes can be calculated quantitatively using time-dependent density functional theory (DFT). Predictive power is obtained from range-separated hybrid functionals using non-empirical tuning of the range-splitting parameter. Excellent performance of this approach is obtained for a series of complexes composed of various aromatic donors and the tetracyanoethylene (TCNE) acceptor, paving the way to systematic non-empirical quantitative studies of charge-transfer excitations in real systems.

5:06PM T36.00014 Transcorrelated method applied to solids: numerical assessment of the SCF effect — KEITARO SODEYAMA, University of Tokyo, KEI SAKUMA, Chiba University, SHINJI TSUJIEYUKI, University of Tokyo — To calculate the electronic structures of solids including electron correlation effects, we have developed the transcorrelated (TC) method which was first proposed by Boys and Handy. In the TC method, the wave function is represented by a correlated wave function FΦ, where Φ is a single Slater determinant and F is a Jastrow function, F = exp[− Σ ij ρij uij]. uij is a two-body function called Jastrow factor. The many-body Hamiltonian H is similarity transformed to an effective Hamiltonian H_TC = F−1HF with up-to-three-body interaction. One-electron orbitals and their orbital energies are optimized by solving a set of Hartree-Fock (HF)-like single particle equations derived by minimizing the variance of the H_TC. In this study, we have investigated the effect of the self-consistent field (SCF) approach which was used in solving the HF-like single particle equations in the TC method. For this purpose, band gaps of Si, SiC, and LiF were calculated as a one-shot perturbation by using the unperturbed LDA orbitals as initial guess orbitals. The difference between the one-shot TC and conventional SCF TC results is small for Si but large for SiC, and especially large for LiF. From this result, we found that the SCF effect was important for strongly polarized solids such as LiF because the initial LDA orbitals were poorly described for such polarized solids.

Wednesday, March 18, 2009 2:30PM - 4:30PM — Session T37 DCP: Focus Session: Structure and Dynamics of Interfacial Water III

2:30PM T37.00001 Study of Water Adsorbed on the Cu(110) Surface using Scanning Tunneling Microscopy and Electron Stimulated Desorption Ion Angular Distribution, JUNSEOK LEE, Department of Chemistry, University of Virginia — The structure of water layer on the Cu(110) surface formed via hydrogen bonding has been investigated with scanning tunneling microscopy (STM), electron stimulated desorption ion angular distribution (ESDIAD), and density functional theory (DFT) calculations. STM results revealed 1D chain and 2D island growth at low temperature (~80 K) and at low coverage regime. ESDIAD results at low coverage indicate that there are two kinds of O-H bonds of water molecules that are pointing out of the surface plane. At higher coverage the two-dimensional islands of water prevail, eventually covering the whole surface at the saturation coverage. Dynamic changes in the structure of the water layer and the local O-H bond direction have also been investigated as a function of annealing temperature. Using DFT calculation, a model of the 1D chain structure will be presented.

3:06PM T37.00002 Theoretical description of excited state dynamics in nanostructures1, ANGEL RUBIO, Nano Bio spectroscopy group and ETSF, Universidad del Pais Vasco and Centro Mixto CSIC-UPV/EHU — There has been much progress in the synthesis and characterization of nanostructures however, there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics, nanoscale opto-electronic devices, light harvesting and emitting nanostructures). We will review the recent implementations of TDDFT to study the optical absorption of biological chromophores, one-dimensional polymers and layered materials. In particular we will show the effect of electron-hole attraction in those systems. Applications to the optical properties of solvated nanostructures as well as excited state dynamics in some organic molecules will be used as text cases to illustrate the performance of the approach. Work done in collaboration with A. Castro, M. Marques, X. Andrade, J.L Alonso, Pablo Echenique, L. Wirtz, A. Marini, M. Gruning, C. Rozzi, D. Varsano and E.K.U. Gross.

1Work supported by Spanish MEC(FIS2007-65702-C02-01), Grupos Consolidados UPV/EHU of the Basque Country Government (IT-319-07) EC e-I3 ETSF and NANOQUANTA projects.

3:42PM T37.00003 Interfacial water in electric field1, ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University (VCU), D. BRATKO, Department of Chemistry, VCU and Department of Chemical Engineering, UC Berkeley, C.D. DAUB, Department of Chemistry, VCU — As accessible experimental length scales become shorter, the modification of interfacial properties of water using electric field (electrowetting) must come to grips with novel effects existing at the nanoscale. I will briefly survey some of our recent progress we have made in understanding these effects using molecular simulations.

1Supported by NSF

3:54PM T37.00004 Molecular Simulation of Reverse Micelles1, JANAMEJAYA CHOWDHARY, BRANKA LADANYI, Department of Chemistry, Colorado State University — Reverse micelles (RM) are surfactant assemblies containing a nanosized water pool dissolved in a hydrophobic solvent. Understanding their properties is crucial for insight into the effect of confinement on aqueous structure, dynamics as well as physical processes associated with solutes in confinement. We perform molecular dynamics simulations for the RM formed by the surfactant Aerosol-OT (AOT) in isooctane (2,2,4-trimethyl pentane) in order to study the effect of reverse micelle size on the aqueous phase. The structure of the RM is quantified in terms of the radial and pair density distributions. Dynamics are studied in terms of the mean squared displacements and various orientational time correlation functions in different parts of the RM so as to understand the effect of proximity to the interface on aqueous dynamics. Shape fluctuations of the RM are also analyzed.

1NSF

4:06PM T37.00005 Ti-O bond distance fluctuations at the hydrated rutile (110) surface, NITIN KUMAR, Department Of Physics, Penn State University, PAUL KENT, ORNL, DAVID COLE, DAVID WESOLOWSKI, Chemical Sciences Division, ORNL, JAMES KUBICKI, Department of Geosciences, The Pennsylvania State University, JORGE SOFO, Department of Physics, The Pennsylvania State University — We studied water on the rutile (110) surface using ab-initio molecular dynamics simulations in NVT ensemble at 280K, 300K, and 320K. Water adsorbs on the 5-fold coordinated titanium atoms or dissociates transferring a proton to a bridging-oxygen atom. The equilibrium between these configurations is dynamical and depends on temperature and water coverage. The titanium-oxygen bond distances at the surface can change as much as 12% depending on the number of hydrogen atoms bonded to oxygen. Hydrogen bonds also affect this distance. A measurement of the Ti-O distance at the surface can be used to estimate the average degree of dissociation. In view of our simulation results, the experimental evidence, such as photoelectron diffraction, indicates a low degree of dissociation under dry conditions.
The TiO$_2$ surface, JIN ZHAO, Dept. of Physics and Astronomy, Univ. of Pittsburgh, KENNETH JORDAN, Dept. of Chemistry, Univ. of Pittsburgh, JINLONG YANG, Hefei Natl. Lab. for Physical Sciences at Microscale, Univ. of Science and Technology of China, HRVOJE PETEK, Dept. of Physics & Astronomy, Univ. of Pittsburgh — At metal-oxide/protic-solvent interfaces, partially hydrated or “wet electron” states represent the lowest energy pathway for electron transfer. Through a joint two-photon photoemission (2PP) experiment and density function theory (DFT) study, we identified the electronic states corresponding to the partially solvated or wet electron state in H$_2$O overlayers on rutile TiO$_2$(110) surface. We find that a network of dangling H atoms can stabilize photoexcited electrons, in so-called wet-electron states. The energies of the “wet electron” states correlate closely with the number and configuration of the dangling H atoms involved in stabilizing them. We also performed DFT calculations of H$_2$O and H covered anatase (101) surface. Comparing with rutile (110), anatase (101) surface accommodates weaker H$_2$O molecule-surface hydrogen bonding. Our calculated wet electron state on anatase (101) surface has a lower energy than on rutile. Moreover, the longer distance between the adjacent adsorbate sites and the lower binding energy of H$_2$O allow for greater freedom for the adsorbed molecules to undergo structural relaxation in solvation of injected electrons. These differences might contribute to the higher photocatalytic activity of anatase compared with rutile. [1] K. Onda B. Li, J. Zhao, K.D. Jordan, J. Yang and H. Petek, Science 308, 1154 (2005).

Wednesday, March 18, 2009 2:30PM - 5:06PM – Session T38 DCP: Focus Session: The Transition State in Physics, Chemistry, and Astrophysics

2:30PM T38.00001 Transition State Theory for Higher-Rank Saddles, GEORGE HALLER, Massachusetts Institute of Technology & Morgan Stanley — Recent developments in transition state theory have lead to a geometric characterization of molecular reactions in phase space. Central to this new characterization is the existence of codimension-one surfaces in the energy shell; these invariant surfaces guide reactiv trajectories through sections of no return, the transition states. The existence of codimension-one invariant surfaces has only been shown in the vicinity of rank-one saddles, i.e., near fixed points with one stable and one unstable direction in addition to neutrally stable directions. For higher-rank saddles, the current framework of geometric transition state theory has remained inapplicable. Here we describe a generalization of the theory to saddles of arbitrary rank. As an application, we describe the nonsequential ionization of helium atoms, a problem with a rank-two saddle.

3:06PM T38.00002 Exploring Topographies and Dynamics on Many-Dimensional Landscapes, R. STEPHEN BERRY, The University of Chicago — A major challenge to understanding and using kinetics is finding the relationships between the topography of the many-dimensional potential energy landscape (or landscapes, for systems with multiple accessible electronic states) and the way that topography, local and large-scale, determines how systems change their structures, relax and anneal. One major difficulty is simply the complexity of the landscape: one is forced to work with small statistical samples of the surface; how should these samples best be chosen? What characteristics of the topography provide the most important information? Another: how does the nature of the interparticle forces determine the topography and hence the character of motion on the surface? And what are the most useful diagnostic tools to tell us about that behavior? We shall address these questions, more in terms of progress toward, rather than providing definitive answers.

3:42PM T38.00003 Transition State Theory: The Phase Space Perspective, TURGAY UZER, Georgia Institute of Technology — Transition State Theory (TST), which is at the basis of chemical reactivity calculations, assumes that once reactants pass through the Transition State, they cannot return. This “no-recrossing” rule serves to define the TS and is a necessary assumption in TST. Conventional transition states always lead to overestimates of the reaction rate because each intersection of the trajectory with the TS counts as a reactive event. Enforcing this no-recrossing condition beyond two degrees of freedom has been the major obstacle to applying TST in multidimensional systems. We will explain the solution of this problem based on dynamical systems theory.

4:18PM T38.00004 Phase Space Transition States for Deterministic Thermostats, GREGORY EZRA, Cornell University, STEPHEN WIGGINS, Bristol University — We describe the relation between the phase space structure of Hamiltonian and non-Hamiltonian deterministic thermostats. We show that phase space structures governing reaction dynamics in Hamiltonian systems, such as the transition state, map to the same type of phase space structures for the non-Hamiltonian isokinetic equations of motion for the thermostatted Hamiltonian. Our results establish a general theoretical framework for analyzing thermostat dynamics using concepts and methods developed in reaction rate theory. Numerical results are presented for the isokinetic thermostat.

4:30PM T38.00005 Using invariant manifolds to classify chaotic transport pathways in mixed phase space, KEVIN MITCHELL, University of California Merced — We describe how the topological structure of stable and unstable manifolds embedded within a chaotic phase space can be used to extract a symbolic classification of chaotic transport and escape pathways. We pay particular attention to phase spaces that contain a mixture of both chaos and regularity. For such systems, the dynamics in the vicinity of “stable islands” is known to be particularly troublesome to analyze. We describe a technique that utilizes the structure of invariant manifolds in the vicinity of such stable islands to extract a symbolic model for the islands’ influence on the transport process. Though our analysis focuses on Hamiltonian systems of two degrees-of-freedom, we also discuss the extension of our technique to higher dimensional phase spaces.

4:42PM T38.00006 Transition State Theory: Variational Formulation, Dynamical Corrections, and Error Estimates, ERIC VANDEN-EIJNDEN, Courant Institute — Transition state theory (TST) is discussed from an original viewpoint: it is shown how to compute exactly the mean frequency of transition between two predefined sets which either partition phase space (as in TST) or are taken to be well separate metastable sets corresponding to long-lived conformational states (as necessary to obtain the actual transition rate constants between these states). Exact and approximate criteria for the optimal TST dividing surface with minimum recrossing rate are derived. Some issues about the definition and meaning of the free energy in the context of TST are also discussed. Finally precise error estimates for the numerical procedure to evaluate the transmission coefficient $\kappa_S$ of the TST dividing surface are given, and it shown that the relative error on $\kappa_S$ scales as $1/\sqrt{\kappa_S}$ when $\kappa_S$ is small. This implies that dynamical corrections to the TST rate constant can be computed efficiently if and only if the TST dividing surface has a transmission coefficient $\kappa_S$ which is not too small. In particular the TST dividing surface must be optimized upon (for otherwise $\kappa_S$ is generally very small), but this may not be sufficient to make the procedure numerically efficient (because the optimal dividing surface has maximum $\kappa_S$, but this coefficient may still be very small).

1We are grateful to the US National Science Foundation for their support of this research.

3Supported by NSF grant PHY-0748828.
The time scale to escape from this metastable state is exponentially large. In both cases, our result fit with experimental measurements pretty well.

When the Gag-Gag attraction is relatively high, the membrane elastic energy provides a kinetic barrier for the two pieces of the partial capsids to merge. This slow and effectively trapped partial budding process, by varying the attractive energy of retroviral proteins (call Gags), relative to the membrane elastic energy.

The budding and assembly is effectively trapped at local free energy minimum, corresponding to a partially budded state. The energy barrier, but a free energy barrier. Energy barriers in biochemical processes are often significant even for reactions proceeding at room temperature因为分子的热运动，使分子不相的势垒成为有效不可逾越。The budding of viruses with varying membrane elasticity creates such a kinetic barrier, as the retroviral proteins (Gag) have higher affinities at higher temperatures. slower budding process is observed, consistent with the experimental observations. This suggests that the budding event is significantly influenced by the membrane elasticity.

The budding and assembly of retroviruses, including HIV, is a complex process that involves the interaction between the viral proteins and the host cell membrane. The budding process is influenced by various factors, including the membrane elasticity, the temperature, and the relative affinities of the viral proteins. Understanding these interactions is crucial for the development of antiviral therapies.

We thank the NIH CHEETAH center grant for financial support.

3:06PM T39.00002 How viral capsids adapt to mismatched cargoes: identifying mechanisms of morphology control with simulations

3:30PM T39.00004 Mechanisms of viral capsid assembly around a polymer

3:42PM T39.00005 Kinetics of human immunodeficiency virus budding and assembly

2:30PM T39.00001 Stochastic modeling of virus capsid assembly pathways

We present a coarse-grained computational model inspired by the assembly of viral capsid proteins around functionalized nanoparticles. With this model, we find parameter values for which subunits faithfully form empty capsids with a single morphology, but adaptively assemble into different icosahedral morphologies around nanoparticles with different diameters. Analyzing trajectories in which adaptation is or is not successful sheds light on the mechanisms by which capsid morphology may be controlled in vitro and in vivo, and suggests experiments to test these mechanisms. We compare the simulation results to recent experiments in which Brome Mosaic Virus capsid proteins assemble around functionalized nanoparticles, and describe how future experiments can test the model predictions.

3:06PM T39.00002 How viral capsids adapt to mismatched cargoes: identifying mechanisms of morphology control with simulations

1Supported by HHMI.

3:18PM T39.00003 The role of protein interactions in HIV-1 Capsid Shape and Stability: A Multiscale Analysis

A coarse grained model of the HIV-1 CA dimer is constructed based on all-atom molecular dynamics simulations of the C-Terminal capsid dimer. Systematic approaches to identify coarse graining sites within the dimer are presented, and the relationship of the coarse grained model parameters to atomistic properties of the capsid discussed. Coarse grained representations of the capsid shell are constructed and their stability examined. The critical importance of an additional carboxyl-hexameric amino terminal interaction is demonstrated. It is shown that this interaction is responsible for generating the curvature of the capsid shell. It is demonstrated that variation of the strength of this interaction for different proteins in the lattice can cause formation of asymmetric, conical shaped closed capsid shells and it is proposed that variations in the structure of the additional carboxyl-amino terminal binding interface during self assembly are critical to capsid cone formation.

3:30PM T39.00004 Mechanisms of viral capsid assembly around a polymer

Mechanisms of viral capsid assembly around a polymer

3:42PM T39.00005 Kinetics of human immunodeficiency virus budding and assembly

The budding of HIV is an essential process that allows the virus to infect new cells. The budding process is influenced by various factors, including the membrane elasticity, the temperature, and the relative affinities of the viral proteins. Understanding these interactions is crucial for the development of antiviral therapies.
3:06PM T39.00007 Exploring the remarkable limits of continuum elastic theory to understand the nanomechanics of viruses. WOUTER ROOS, Natuur- en Sterrenkunde, Vrije Universiteit, Amsterdam, MELISSA GIBBONS, WILLIAM KLUG, Department of Mechanical and Aerospace Engineering, UCLA. GIJS WUITE, Natuur- en Sterrenkunde, Vrije Universiteit, Amsterdam — We report nanindentation experiments by atomic force microscopy on capsids of the Hepatitis B Virus (HBV). HBV is investigated because its capsids can form in either a smaller T=3 or a bigger T=4 configuration, making it an ideal system to test the predictive power of continuum elastic theory to describe nanometre-sized objects. It is shown that for small, consecutive indentations the particles behave reversibly linear and no material fatigue occurs. For larger indentations the particles start to deform non-linearly. The experimental force response fits very well with finite element simulations on coarse grained models of HBV capsids. Furthermore, this also fits with thin shell simulations guided by the Föppl-von Kármán (FvK) number (the dimensionless ratio of stretching and bending stiffness of a thin shell). Both the T=3 and T=4 morphology are very well described by the simulations and the capsid material turns out to have the same Young’s modulus, as expected. The presented results demonstrate the surprising strength of continuum elastic theory to describe indentation of viral capsids.

4:18PM T39.00008 to be determined by you. JAMES CONWAY, TBD — No abstract available.

4:54PM T39.00009 Conformational changes of Gag HIV-1 on a lipid bilayer measured by neutron reflectivity provides insights into viral particle assembly. ROBBIN BRUINSMA, JOSEPH RUDNICK, Dept of Physics and Astronomy, UCLA. — The self-assembly of the protein shell (“capsid”) of a virus is believed to obey the Law of Mass Action (LMA) despite the fact that viral assembly is not a reversible process. In this paper we examine a soluble model for irreversible capsid assembly, the “Assembly-Line Model.” We show that, in this model, viral assembly from a supersaturated solution is characterized by a shock front propagating in the assembly configuration space from small to large aggregate sizes. If this shock front is able to reach the size of an assembled capsid, then transient state develops characterized by a “pseudo” LMA. This pseudo LMA describes partitioning of capsid proteins between assembled capsids and a metastable, supersaturated solution of free proteins that decays logarithmically slowly. We show that the line energy of assembly intermediates is the key parameter that determines this metastable state.

5:18PM T39.00011 A comparison of the elastic moduli of an animal and plant virus. D. GUI, X. CHEN, A.L.N. RAO, S. GILL, U. MOHIDDEEN, R. ZANDI, University of California, Riverside, CA — We have used Atomic Force Microscopy (AFM) to image single Sindbis and BMV viruses. The AFM was then used in force spectroscopy mode to measure their elastic Modulii. The similarities and differences will be discussed.

Wednesday, March 18, 2009 2:30PM - 5:06PM — Session T40 DBP: Focus Session: Knots and Loops in Biomolecules

2:30PM T40.00001 Dodging the crisis of folding proteins with knots. JOANNA SUŁKOWSKA, University of California, San Diego — Proteins with nontrivial topology, containing knots and slipknots, have the ability to fold to their native states without any additional external forces invoked. A mechanism is suggested for folding of these proteins, such as YbK and YbA, which involves an intermediate configuration with a slipknot. It elucidates the role of topological barriers and backtracking during the folding event. It also illustrates that native contacts are sufficient to guarantee folding in around 1-2% of the simulations, and how slipknot intermediates are needed to reduce the topological bottlenecks. As expected, simulations of proteins with similar structure but with knot removed fold much more efficiently, clearly demonstrating the origin of these topological barriers. Although these studies are based on a simple coarse-grained model, they are already able to extract some of the underlying principles governing folding in such complex topologies.

3:06PM T40.00002 Size and Shape of Knotted Polymers. ERIC RAWDON, University of St. Thomas — We use numerical simulations to investigate how the size and bulk of a filament change when it is self-avoiding, where the self-avoiding property is the main effect of knotting. In particular, we analyze different types of geometric containers that enable polymer configurations and describe the similarities and differences between them. This work has been done in collaborations with Akos Dobay, John Kern, Kenneth Millett, Michael Piatek, Patrick Plunkett, and Andrzej Stasiak.

3:18PM T40.00003 On the geometry of stiff knots. OLIVIER PIERRE-LOUIS, Oxford Theoretical Physics and LSP, Univ. J.Fourier, Grenoble — We report on the geometry and mechanics of knotted strings. We focus on the situation where the string is stiff (it has a large bending rigidity), and thin (its width is much smaller than its length). We find that: (i) the equilibrium energy depends on the type of knot as the square of the bridge number; (ii) braid localization is a general feature of stiff strings entanglements; (iii) there is an upper bound for the multiplicity of the braids and contact points in the ground state. (iv) Finally, a general confinement inequality is used to derive an upper bound on the knot gyration radius. We shall also discuss the asymptotic behavior of the knot when the filament width is small, both in the presence and in the absence of torsion (twist) energy. We conjecture a universal ground state geometry for thin strings with torsion rigidity in the presence of a large twists. Ref: R. Gallotti, O. Pierre-Loius, Phys. Rev. E 75, 031801 (2007).
3:30PM T40.00004 Conformation and Dynamics of Linear Chains, Circular and Partial Loops, JEN-FANG CHANG, Institute of Physics, Academia Sinica, YENG-LONG CHEN, Institute of Physics & Research Center for Applied Science, Academia Sinica. POLYMER PHYSICS & COMPLEX FLUIDS TEAM — Recent single molecule experiments have reported the diffusivity ratio between circular and linear DNA of the same molecular weight to be 1.3, between the ratio predict by renormalization group theory (1.45) and classical Kirkwood theory (1.18). In earlier light and neutron scattering measurements of synthetic polymers, the ratio has been reported to be around 1.1-1.2. Our work employs the Lattice-Boltzmann method with Brownian dynamics to examine the diffusivity ratio for a long chain (N=320). We also examined partially closed loops that are half-closed, quarter-closed, and eighth-closed with the same contour length. Just surprisingly, we find that the loop with the smallest radiiuses of gyration and the highest diffusivity is not the fully closed (circular) loop, but a partially-closed one.

3:42PM T40.00005 Modeling the behavior of DNA-loop-extruding enzymes, ELNAZ A. BAUM-SNOW, JOHN F. MARKO, Northwestern University — Condensins proteins are large complexes belonging to a family of ATP hydrolyzing proteins known as SMC (Structural Maintenance of Chromosomes). Condensins are believed to play a vital role in chromosomal assembly and segregation in eukaryotic cells but the details of their function along chromatin are poorly understood. Here, we propose a model to describe the behavior of DNA-loop-extruding proteins, such as type I restriction enzymes, which we believe can be used to understand condensin’s function. We assume an effective motor behavior for these enzymes in which the bias of the two dimer heads is to travel away from each other, which results in loop formation along the DNA lattice. Processivity causes the enzymes to stack on top of each other. We further discuss the results of theory and computer simulations for different values of motor bias and processivity.

3:54PM T40.00006 Intricate knots in proteins: statistics, function and evolution, PETER VIRNAU, Johannes Gutenberg University Mainz — Protein knots, mostly regarded as intriguing oddities, are gradually being recognized as significant structural motifs. These elusive knots are present in the backbone of only about 1 in 200 proteins. It is by and large unclear how these exceptional structures actually fold, and only recently, experiments and simulations have begun to shed some light on this issue. In this talk I will present an overview of these peculiar structures from the current version of the Protein Data Bank and discuss some particularly intriguing examples of this set as well as evolutionary and functional implications.

4:30PM T40.00017 The Role of Entropic Effects on DNA Loop Formation, DAVID WILSON, U of Michigan, ALEXEI TRACHENKO, University of Michigan, TODD LILLIAN, NOEL PERKINS, JENS CHRISTIAN MEINERS, University of Michigan — The formation of protein mediated DNA loops often regulates gene expression. Typically, a protein is simultaneously bound to two DNA operator sites. An example is the lactose repressor which binds to the Lac operator of E. coli. We characterize the mechanics of this system by calculating the free energy cost of loop formation. We construct a Hamiltonian that describes the change in DNA bending energy due to linear perturbations about the looped and open states, starting from a non-linear mechanical rod model that determines the shape and bending energy of the inter-operator DNA loop while capturing the intrinsic curvature and sequence-dependent elasticity of the DNA. The crystal structure of the Lac protein provides the boundary conditions for the DNA. We then calculate normal modes of the open and closed loops to account for the thermal fluctuations. The ratio of determinants of the two Hamiltonians yields the partition function, and the enthalpic and entropic cost of looping. This calculation goes beyond standard elastic energy models because it fully accounts for the substantial entropic differences between the two states. It also includes effects of sequence dependent curvature and stiffness and allows anisotropic variations in persistence length. From the free energy we then calculate the J-factor and ratio of loop lifetimes.

4:42PM T40.00008 Helical growth trajectories in plant roots interacting with stiff barriers, SHARON GERBODE, Physics Department, Cornell University, ROSLYN NOAR, MARIA HARRISON, Boyce Thompson Institute for Plant Research, Cornell University — Plant roots successfully navigate heterogeneous soil environments with varying nutrient and water concentrations, as well as a variety of stiff obstacles. While it is thought that the ability of roots to penetrate into a stiff lower soil layer is important for soil erosion, little is known about how a root actually responds to a rigid interface. We have developed a laser sheet imaging technique for recording the 3D growth dynamics of plant roots interacting with stiff barriers. We find that a root encountering an angled interface does not grow in a straight line along the surface, but instead follows a helical trajectory. These experiments build on the pioneering studies of roots grown on a tilted 2D surface, which reported “root waving,” a similar curved pattern thought to be caused by the root’s sensitivity to both gravity and the rigid surface on which it is grown. Our measurements extend these results to the more physiologically relevant case of 3D growth, where the spiral trajectory can be altered by tuning the relative strengths of the gravity and touch stimuli, providing some intuition for the physical mechanism driving it.

4:54PM T40.00009 The Penrose-Hameroff Orchestrated Objective-Reduction Proposal for Human Consciousness is Not Biologically Feasible, JEFFREY REIMERS, LAURA MCKEMMISH, NOEL HUSH, The University of Sydney, ROSS MCKENZIE, ALAN MARK, The University of Queensland — Penrose and Hameroff have argued that conventional models of brain function based solely on neural linear-computational elements cannot account for human consciousness, claiming instead that quantum-computation elements are required. We construct a Hamiltonian that describes the change in DNA bending energy due to linear perturbations about the looped and open states, starting from a non-linear mechanical rod model that determines the shape and bending energy of the inter-operator DNA loop while capturing the intrinsic curvature and sequence-dependent elasticity of the DNA. The crystal structure of the Lac protein provides the boundary conditions for the DNA. We then calculate normal modes of the open and closed loops to account for the thermal fluctuations. The ratio of determinants of the two Hamiltonians yields the partition function, and the enthalpic and entropic cost of looping. This calculation goes beyond standard elastic energy models because it fully accounts for the substantial entropic differences between the two states. It also includes effects of sequence dependent curvature and stiffness and allows anisotropic variations in persistence length. From the free energy we then calculate the J-factor and ratio of loop lifetimes.

Wednesday, March 18, 2009 2:30PM - 5:30PM — Session T41 DMP DCMP: Ferroelectricity and Structural Phase Transitions 413

2:30PM T41.00001 Strained enabled Ferroelectricity in CaTiO$_3$ Thin Films Probed by Non-linear Optics and Scanning Probe Microscopy, EFTIHIA VLHASO, AMIT KUMAR, SAVA DENEV, CHARLES BROOKS, Materials Science and Engineering, Pennsylvania State University, DARRELL SCHLOM, Materials Science and Engineering, Cornell University, CARL-JOHAN EKLUND, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University, CRAIG J. FENNIE, Applied and Engineering Physics, Cornell University, VENKATARAMAN GOPALAN, Materials Science and Engineering, Pennsylvania State University — Calcium titanate, CaTiO$_3$, is not a ferroelectric in its bulk form. However, first principles calculations predict that biaxially tensile strained CaTiO$_3$ thin films should become ferroelectric. Here, we indeed confirm that strained CaTiO$_3$ films become ferroelectric with a Curie temperature of ~125K. Optical second harmonic generation (SHG) measurements, polarization studies, and in-situ electric-field measurements for a number of films with different strain values will be presented: CaTiO$_3$/DyScO$_3$(110), CaTiO$_3$/SrTiO$_3$(100), CaTiO$_3$/GdScO$_3$/NdGaO$_3$(110). CaTiO$_3$/LaSrAlO$_3$(001) as well as for a single crystal CaTiO$_3$. From these studies, we conclude that strained CaTiO$_3$ films are ferroelectric with a point group symmetry of mm2, and show reversible domain switching characteristics under an electric field. We also present results of variable temperature piezoelectric force microscopy for imaging the polar domains in the ferroelectric phase. These results suggest that strain is a valuable tool for inducing polar, long range ferroelectric order in even non-polar ceramic materials such as CaTiO$_3$. 
2:42PM T41.00002 Potential and piezoelectric response imaging of 180° domain of atomically ordered clean surfaces of BaTiO₃ single crystals in UHV, YUKIO WATANABE, Kyushu University, S. KAKU, D. MATSUMOTO, S.W. CHEONG, Rutgers Uinn. — We report the electrostatic and piezoelectric properties of the clean, free surface of BaTiO₃ single crystal in ultra high vacuum (UHV). The topographic imaging by AFM confirmed that the surface is atomically wellordered exhibiting clear one-lattice-height atomic steps. The amplitude and the phase image of piezoelectric response microscopy (PFM) identified 180° domains. The electrostatic potential mapping by Kelvin force microscopy (KFM) of these domains revealed that the shapes of the domains agreed exactly with the PFM images, which confirms the correctness of the standard 180° domain theory and agrees with closure domains. However, the potential difference of upward and downward domain is approx. 0.1V, which is 100 times smaller than the value estimated by the standard theory. Similar measurements with changing temperature across Curie temperature show that this result cannot be explained by the compensation of the spontaneous polarization by contamination or oxygen deficiency or ionic conduction. The present results suggest that an intrinsic electrostatic shielding mechanism exists for 180° domains, which is consistent with the reports of surface electron/ hole layers [1].


2:54PM T41.00003 Magnetic Color Symmetry of Lattice Rotations in a Non-magnetic Material, SAVA DENEV, A. KUMAR, M. D. BIELGALSKI, Pennsylvania State University, H. W. JANG, C. M. FOLKMAN, University of Wisconsin-Madison, A. VASUDEVARAO, Pennsylvania State University, Y. HAN, I. M. REANEY, University of Sheffield, S. TROLLEY-MCKINSTRY, Pennsylvania State University, C.-B. EOM, University of Wisconsin-Madison, D. G. SCHLOM, V. GOPALAN, Pennsylvania State University — Oxygen octahedral rotations are the most common phase transitions in perovskite crystal structures. Here we show that the color symmetry of such pure elastic distortions is isomorphic to magnetic point groups, which allows their probing through distinguishing polar versus magnetic symmetry. We demonstrate this isomorphism using nonlinear optical probing of the octahedral rotational transition in a compressively strained SrTiO₃ thin film that exhibits ferroelectric (4mm) and antiferrodistortive (1′4mn) phases evolving through independent phase transitions. The approach has broader applicability for probing materials with lattice rotations that can be mapped to color groups.

3:06PM T41.00004 Spontaneous polarization and piezoelectricity in polar molecular crystals, IVO BORRIELLO, University of Naples Federico II, Naples Italy, GIOVANNI CANTELE, CNR-COHERENTIA, University of Naples Federico II, Naples Italy, DOMENICO NINNO, GIUSEPPE IADONISI, University of Naples Federico II, Naples Italy — Molecular materials with a polar arrangement of the constituent dipoles are good candidates for exhibiting piezoelectric properties, directly related to the strain-induced polarization. The metal-organic molecular crystal (4-dimethylaminopyridyl)bis(acylacetato)zinc(II) (ZND) has been investigated from first principles. The spontaneous polarization and the piezoelectric properties have been studied by means of the modern theory of polarization, focusing on the relation between the piezoelectric properties of the organic crystal and the electronic properties of the polar molecule.

3:18PM T41.00005 Interfaces in ferroelastics: fringing fields, scaling, size and shape effects, TURAB LOOKMAN, Los Alamos National Laboratory — We consider the problem of determining the elastic fields and microstructure within a transformable region of size L, in which structural transformations from a parent to a product phase with variants can occur, that is surrounded by a fixed parent matrix. By demanding mechanical equilibrium and strain compatibility at the parent-product interface, we demonstrate that for sufficiently coarse twins the width of the twinned product phase varies as sqrt(L), but this breaks down if L is small enough for the surface and bulk energies to compete. As L decreases further, a transition to a stable checkboard pattern containing the parent and product variants occurs and this subsequently disappears if L is too small. We relate our findings to the behavior of transformations in nanograins of NiTi within an amorphous matrix and nanoscale checkboard microstructure seen in inorganic spinels. Understanding how microstructure emerges from a given configuration of interfaces is a non-trivial task and our overarching theme is to study the interplay of orientations, decaying strain fields, length scaling of energy and dependence of transition on size and shape of a transformable region within a parent matrix.

3:30PM T41.00006 Local Polarization Dynamics and Bias-Induced Phase Transitions in Ferroelectric Relaxors: Time-resolved Spectroscopy and Ergodic Gap Mapping, S.V. KALININ, B. RODRIGUEZ, M.P. NIKIFOROV, N. BALKE, S. JESSE, O.S. OVCHINNIKOV, A.A. BOKOV, Z.-G. YE, ORNL TEAM, SIMON FRAZER UNIV. TEAM — Mesoscopic domain structure and dynamics in PMN-PT sols solutions is studied using spatially resolved time- and voltage spectroscopic imaging modes. For compositions close to the MPB, we observe the formation of classical ferroelectric domains with rough self-affine boundaries. In the ergodic phase (PMN and PMN-10PT), the region of size L, in which structural transformations from a parent to a product phase with variants can occur, that is surrounded by a fixed parent matrix.

3:42PM T41.00007 Field Dependence of Glassy Freezing in a Relaxor Ferroelectric, MATTHEW DELGADO, EUGENE COLLA, MICHAEL WEISSMAN, University of Illinois at Urbana-Champaign, PHILIP GRIFFIN, University of Tennessee — Magnetic susceptibility measurements on the cubic relaxor ferroelectric (PbMg₁/₃Nb₂/₃O₃)₀.₉₈(PbTiO₃)₀.₁₂ were performed at various DC electric field strengths applied along the [111] direction. The temperature-frequency-dependencies fits the Vogel-Fulcher form, allowing the extraction of a frequency-independent glassy freezing temperature. These Vogel-Fulcher temperatures showed significant reductions in applied fields, following an empirical Gabay-Toulouse form, similar to vector spin glasses. The magnitude of the sensitivity indicates that the glassy state is formed by interactions among the same entities that account for the susceptibility, i.e. the polar nanoregions. This interpretation is supported by data on a powder sample of PbMg₁/₃Nb₂/₃O₃ (PMN), with grains too small to support large-scale inter-nanoregion cooperativity, in which the Vogel-Fulcher behavior is lost [1]. [1] J. Carreau et al., Appl. Phys. Lett. 92, 242902 (2008).

[1]Work performed in collaboration with M. Porta, T. Castan, P. Lloveras (U. of Barcelona), A. Saxena (LANL) and S. Shenoy (U. of Hyderabad).

3:54PM T41.00008 The three characteristic Temperatures of Relaxor Dynamics and their Meaning, JEAN TOULOUSE, Lehigh University — In this report, we compare the temperature evolution of several physical properties of the relaxor systems PZN, PMN and KTN. We show that three rather than two characteristic temperatures can be identified, Tₚ, T⁺ and T⁻, and discuss their meaning in light of dielectric, Raman and neutron scattering experimental results.

[2]This work is supported by the US Department of Energy under grant DE-FG02-06ER46318.
Ridge National Laboratory, USA — The transition metal dihydride TiH
study
we provide evidence for the presence of a continuous martensitic transition in the binary AuZn system. In AuNi,Zn, elastic neutron scattering
detects new commensurate Bragg peaks (modulation) appearing at \( Q = (1.33, 0.67, 0) \) at temperatures corresponding to each sample’s martensitic transition
temperature, \( T_M \). The pressure dependence of the transition in each alloy, shows a low-temperature saturation of the order parameter (strain-shuffle) that leads
to highly non-linear phase boundaries in temperature-pressure space and to superconductivity in the case of AuNi,Zn.

1 Work performed under the auspices of the U.S. D.O.E.

18PM T41.00010 First principles determination of phase transitions in magnetic shape memory alloys\(^1\), TILMANN HICKEL, MPI fuer Eisenforschung GmbH, MATTHE JUITTEWAAL, JOERG NEUGEBAUER — Magnetic shape memory alloys have recently attracted a lot of excitement, since they allow shape changes of more than 10% with a frequency in the kHz regime. The fundamental origin of this effect is related to a martensitic phase transition. The material system Ni\(_2\)MnGa is the most promising candidate for applications, but its operation temperatures and ductility still need to be improved. Hence, an extension of the currently very limited knowledge on the phase diagram is decisive. In order to identify the stable structures and their transitions we performed ab initio calculations of free energies for the austenite, the (modulated) pre-martensite and the unmodulated martensite. Quasiharmonic phonons and fixed-spin magnons are considered, employing density functional theory. Using this approach we were able to successfully describe the phase transition in detail, to reveal the involved delicate interplay of vibrational and magnetic excitations and to accurately
determine the transition temperature. The methods are used to interpret the experimental findings and to make predictions for modified material compositions.

4:30PM T41.00011 A fluctuation-based probe to criticality in structural transitions , U. CHANDNI, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560 012, H.S. VIJAYA, S. MOHAN, Department of Instrumentation, Indian Institute of Science, Bangalore 560 012 — Many natural phenomena, extending from biology to material science, involve slowly driven dissipative systems that are far from thermal equilibrium, triggered only by a slowly varying external field and to which the systems respond through scale-free avalanches in physical observables. In spite of decades of research, experiments are inconclusive whether these systems self organize to the critical state over a broad range of external field, or if there exists a unique critical point that is smudged by a wide critical zone. Here, through the higher order statistics of time dependent avalanches, or noise, in electrical resistivity during temperature-driven martensite transformation in thin nickel-titanium films, we demonstrate for the first time, the existence of a singular 'global instability' or divergence of the correlation length as a function of temperature. These results not only establish a mapping of non-equilibrium first order phase transition and equilibrium critical phenomena, but perhaps also call for a re-evaluation of many existing experimental claims of self-organized criticality. References: 1. U. Chandni et al, Appl. Phys. Lett. 92, 112110 (2008) 2. U. Chandni et. al, arXiv:0811.0102 (2008).

4:42PM T41.00012 Structural transformations and dislocations within the Landau theory , ROMAN GRÖGER, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National Laboratory — We propose a two-dimensional model (Gröger et al., PRB76:194101, 2008) that demonstrates how the Landau theory of first order phase transitions can be coupled with plasticity. It is based on Kröner’s continuum theory of dislocations that views each dislocation as a source of incompatibility between the components of the elastic strain tensor. This incompatibility then couples to the order parameter that is a local representation of the space group of the crystalline lattice. The order parameter field is obtained by minimizing the free energy and this provides both the stress fields and the Peach-Koehler forces on individual dislocations. The evolution of the dislocation density is then obtained by a Fokker-Planck equation. Updating the dislocation density results in a new estimate of the distribution of strain incompatibilities and this serves as an input to the subsequent minimization of the free energy. This self-consistent procedure thus allows for a simultaneous evolution of the order parameter texture and the density of dislocations. To develop a clear link between the microscopic and mesoscopic dislocation density, the crystal dislocations in individual slip systems are restricted to glide in their well-defined slip planes. Upon cooling, the finite dislocation density gives rise to heterogeneous nucleation of the martensite and thus results in a shift of the transformation temperature.

5:45PM T41.00013 Spontaneous phase transition of nano-sized boron nitride – A quantum size effect , HONGLI DANG, University of Tulsa, Y.G. SHEN, City University of Hong Kong, SANWU WANG, University of Tulsa — We report first-principles quantum-mechanical calculations that predict a novel phase transition of nano-sized boron nitride (BN) thin-films. When the thickness of the BN film is below 1.4 nm, a spontaneous phase transition from the diamond-like structure to a graphite phase is predicted. The process would involve no energy barrier. When the thickness of the film increases, on the other hand, energy barriers for the phase transition would appear and gradually increase with the thickness. Calculations show that while the graphite structure has a lower total energy than the corresponding diamond-like structure for the BN thin-film with any thickness, the spontaneous phase transition would occur only when the size is small. We attribute this phenomenon to the quantum size effect.

3Supported in part by the NSF (CMMI-0645953), by the NSF’s TeraGrid resources provided by the National Center for Supercomputing Applications (TG-DMR080005N), and by the National Center for Computational Sciences at Oak Ridge National Laboratory.

5:06PM T41.00014 High Pressure Studies of the Metal-Insulator Transition in Pure NiS\(_2\) , ARNAB BANERJEE, YEJUN FENG, RAFAEL JARAMILLO, THOMAS F. ROSENBAUM, James Frank Institute, The University of Chicago, APS, ANL, SECTOR 4 AND 6 TEAM, JOE PLUTH/ANL APS SECTOR 13 COLLABORATION — Ni(S,Se)\(_2\) is one of the few Mott-Hubbard systems where a structural phase transition does not preclude quantitative study of the localization of charge at the \( T = 0 \) metal-insulator transition. Using diamond anvil cell techniques, we study the corresponding behavior of pure NiS\(_2\) at its quantum critical point. We characterize the electronic, magnetic and structural behavior of this model system through a combination of transport and synchrotron scattering techniques, with a particular interest in the effects of disorder at a quantum phase transition.

5:18PM T41.00015 Effect of pressure on the tetragonal distortion in TiH\(_2\) : a first-principles study , R. DE COSS, R. QUIJANO, Department of Applied Physics, Cinvestav-Merida, A.P. 73 Cordemex 97310 Merida, Yucatan, Mexico, D.J. SINGH, Oak Ridge National Laboratory, USA — The transition metal dihydride TiH\(_2\) present the fluoride structure (CaF\(_2\)) at high temperature but undergoes a tetragonal distortion with \( c/a < 1 \) at low temperature. Early electronic band structure calculations have shown that TiH\(_2\) in the cubic phase display a nearly flat double degenerated band at the Fermi level. Thus the low temperature tetragonal distortion has been associated to a Jahn-Teller effect. Nevertheless, recently we have show that the instability of fcc-TiH\(_2\) is likely to be related with a van Hove singularity. In the present work, we have performed ab-initio calculations of the electronic structure and the tetragonal distortion for TiH\(_2\) under pressure (0-30 GPa). We found that the fcc-fct energy barrier and the tetragonal distortion increases with pressure. The evolution of the tetragonal distortion is analyzed in terms of the electronic band structure. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 49985.
In the past decade, the study of our Universe has entered a data-driven era. Indeed, observational advances indicate that cosmologists can understand the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics. Cosmologists have mapped out the relic radiation from the big bang itself and have succeeded in enormous projects to map the patterns of galaxies and the evolution of our Universe in exquisite detail and use our Universe as a laboratory with which to make profound statements about the laws of physics.
gene brushes, and implemented a two-stage transcription/translation cascade. Highly sensitive to DNA density, orientation and composition. As a step towards multi-gene synthetic systems, we integrated on a chip two spatially separated brushes coding for entire genes on a surface by means of a new photolithographic approach. The gene density can be controlled from dilute to high density where the local concentration – Megabase pairs per micron cubed – is comparable to that in a bacterium. The gene brush, therefore, emulates the crowded systems of Maryland — No abstract available.

M. C. Choi at al, PNAS 2004, 101, 17340-17344
M.C Choi at al, Macromolecules 2005, 38, 9882-9884
This work was done with C. R. Safinya's group at UCSB and Hee-Tae Jung's group at KAIST.

1D biaxially confined regime with the effective persistence length. We were able to generate defect domains that are nearly uniformly arranged in 2D ordered structures by using the structure of smectic liquid in the microchannels. We found that the F-actin undergoes a transition from a 2D randomly oriented regime to a 1D biaxially confined regime with the effective persistence length. We were able to generate defect domains that are nearly uniformly arranged in 2D ordered patterns by controlling the surface hydrophobicity. Furthermore, the formation of a large-area ordered structure of toric focal conic domains was generated. This work was done with C. R. Safinya’s group at UCSB and Hee-Tae Jung’s group at KAIST.

2. M. C. Choi at al, PNAS 2004, 101, 17340-17344

9:12AM V1.00003 to be determined by you, XIAO-LUN WU, Univ.of Pittsburgh — No abstract available.

9:48AM V1.00004 to be determined by you, SUI HUANG, Institute for Biocomplexity and Informatics — No abstract available.

10:24AM V1.00005 Activity-dependent stochastic resonance in recurrent neuronal networks, VLADISLAV VOLMAN, UCSD — An important source of noise for neuronal networks is that of the stochastic nature of synaptic transmission. In particular, there can occur spontaneous asynchronous release of neurotransmitter at a rate that is strongly dependent on the presynaptic Ca2+ concentration and hence strongly dependent on the rate of spike induced Ca2+. Here it is shown that this noise can lead to a new form of stochastic resonance for local circuits consisting of roughly 100 neurons - a "microcolumn"- coupled via noisy plastic synapses. Furthermore, due to the plastic coupling and activity-dependent noise component, the detection of weak stimuli will also depend on the structure of the latter. In addition, the circuit can exhibit short-term memory, by which we mean that spiking will continue to occur for a transient period following removal of the stimulus. These results can be directly tested in experiments on cultured networks.

This research has been supported by the NSF-sponsored Center For Theoretical Biological Physics (grant nos. PHY-0216576 and PHY-0225630).

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V2 DCMP DPOLY: Constrained Polymers Spirit of Pittsburgh Ballroom BC

8:00AM V2.00001 The low-force elasticity of single-stranded DNA, OMAR A. SALEH, Materials Dept., UCSB — Single-molecule manipulation experiments, in which a single polymer is stretched with a known force while its extension is measured, are typically described by ideal models (e.g. the worm-like chain or freely-jointed chain) that account only for the polymer’s local stiffness, but ignore long-range ‘excluded-volume’ interactions. Yet, the basic (and successful) Flory scaling theory indicates that long-range interactions must be included to describe the zero-force self-avoiding walk structure of a polymer. Here, we reconcile single-molecule force-extension data with scaling theories of polymer elasticity: measurements of denatured single-stranded DNA show a regime where the extension grows as a non-linear power law with force, in accord with previously-unproven ‘tensile blob’ models. Analysis of the salt dependence of this regime indicates that the polymer’s Kuhn length is proportional to the Debye length. This contradicts the classic Odijk-Školnick-Fixman theory; I will discuss possible explanations for this discrepancy.

8:36AM V2.00002 Confinement Effects on the Structure of Complex Fluids, MAHN KIM, KAIST — Actin is a key component of the protein complex responsible for producing contractile force in skeletal muscle. Filamentous actin, called F-actin, is a two-stranded helical protofilament with a diameter of ~8nm and a contour length of ~10m. The experimental results show that the persistence length of the F-actin is 4 -20 m. One of interesting problems is to find the structure of a semiflexible filament in a confined space [1], such as a channel width less than the persistence length. The other interesting problem is to find the surface treatment effect on the liquid crystal structure in a confined space. The boundary conditions imposed by the walls of the microchannel generate the spatial patterning of defect domains in a smectic liquid crystal [2] and the formation of a large-area ordered structure [3] by using the structure of smectic liquid in the microchannels. We found that the F-actin undergoes a transition from a 2D randomly oriented regime to a 1D biaxially confined regime with the effective persistence length. We were able to generate defect domains that are nearly uniformly arranged in 2D ordered patterns by controlling the surface hydrophobicity. Furthermore, the formation of a large-area ordered structure of toric focal conic domains was generated. This work was done with C. R. Safinya’s group at UCSB and Hee-Tae Jung’s group at KAIST.


9:12AM V2.00003 Is your brain wired optimally?, DMITRI CHKLOVSKII, Janelia Farms — No abstract available.

9:48AM V2.00004 Gene brushes on a chip: From crowding and the search problem to synthetic systems, ROY BAR-ZIV, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, 76100, Israel — We assemble DNA polymer brushes coding for entire genes on a surface by means of a new photolithographic approach. The gene density can be controlled from dilute to high density where the local concentration - Megabase pairs per micron cubed – is comparable to that in a bacterium. The gene brush, therefore, emulates the crowded medium of the cell, allowing us to study DNA transactions in vitro under native conditions. We find that transcription/translation from these gene brushes is highly sensitive to DNA density, orientation and composition. As a step towards multi-gene synthetic systems, we integrated on a chip two spatially separated gene brushes, and implemented a two-stage transcription/translation cascade.

10:24AM V2.00005 Confinement effects on folding of proteins and RNA, DEV THIRUMALAI, University of Maryland — No abstract available.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V3 DCMP DAMOP: Correlated Phases in Fermi Gases of Ultracold Atoms 301/302

8:00AM V3.00001 A Mott insulator of fermionic atoms in an optical lattice, HENNING MORITZ, ETH Zurich — In a solid material strong interactions between the electrons can lead to surprising properties. A prime example is the Mott insulator, where the suppression of conductivity is a result of interactions and not the consequence of a filled Bloch band. The proximity to the Mott insulating phase in fermionic systems is the origin for many intriguing phenomena in condensed matter physics, most notably high-temperature superconductivity. Compared to real materials, a fermionic quantum gas trapped in an optical lattice offers a very pure realisation of the Hubbard model, giving a new approach to understand the physics of strongly correlated systems. We report on the formation of a Mott insulator of a repulsively interacting two-component Fermi gas in an optical lattice. It is signalled by three features: a drastic suppression of doubly occupied lattice sites, a strong reduction of the compressibility inferred from the response of double occupancy to atom number increase, and the appearance of a gapped mode in the excitation spectrum. In collaboration with Robert Jördens, Niels Strohmaier, and Daniel Greif, ETH Zurich; Kenneth Günter, ETH Zurich, ENS Paris; Leticia Tarruell and Tilman Esslinger, ETH Zurich.
8:36AM V3.00002 The phase-diagram of a superfluid two-component Fermi gas1. WOLFGANG KETTERLE, Research Laboratory for Electronics, MIT-Harvard Center for Ultracold Atoms, and Department of Physics, MIT, Cambridge, MA 02139 — What is the benefit of realizing superfluidity in a gas a million times more dilute than air? Such systems consist of well-separated atoms which can be observed and manipulated with the control and precision of atomic physics, and which can be treated with first-principles calculations. By implementing scattering resonances, we have realized the strong-coupling limit of the Bardeen Schrieffer-Cooper (BCS) mechanism and observed a normalized transition temperature of 20% of the Fermi temperature, higher than in any superconductor. When the population of the two spin states is imbalanced, pairing is frustrated, and superfluidity is quenched at the Chandrasekhar-Clogston limit. When the fermions can form molecules, we observe the emergence of bosonic behavior, and an imbalanced two-component Fermi system can be described as a boson-fermion mixture. Pairing correlations have been studied by rf spectroscopy, determining the fermion pair size and the pairing gap energy in a resonantly interacting superfluid. These studies illustrate a new approach to condensed-matter physics where many-body Hamiltonians are realized in dilute atomic gases.

1Work done in collaboration with Yong-Il Shin, Andre Schirotzek and Christian Schunck.

9:12AM V3.00003 Trapping and cooling fermionic atoms into the Mott and Néel states1, CORINNA KOLLATH, CPHT, Ecole Polytechnique, CNRS, 91128 Palaiseau, France — Atomic gases cooled to Nanokelvin temperatures are a new exciting tool to study a broad range of quantum phenomena. In particular, the outstanding degree of control which has been achieved over these quantum systems facilitates access to strongly correlated quantum many body physics. For example, optical lattices have been created to mimic condensed matter systems. We perform a theoretical study of a fermionic gas with two repulsively interacting hyperfine states confined to an optical lattice. We determine a generic state diagram in the presence of a harmonic confining potential. We discuss implications for current experiments. Further we outline different strategies to reach the antiferromagnetic phase.

1L. De Leo, A. Georges, M. Ferrero, O. Parcollet

9:48AM V3.00004 Polarized Fermi condensates, MEERA PARISH, Princeton University — We theoretically investigate the polarized two-component Fermi gas, which is the simplest fermion system displaying both superfluidity and “magnetism”. In particular, we show that the elusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) modulated superfluid phase may be realized by embedding the polarized Fermi gas in an array of weakly-coupled parallel 1D “tubes” produced by a two-dimensional optical lattice. We argue that the most promising regime for observing the FFLO phase is in the quasi-1D regime, where the atomic motion is largely 1D but there is weak tunneling in the transverse directions that stabilizes long range order. Moreover, within this system, there is an additional phase transition in the FFLO phase, where the quasiparticle spectrum changes from gapless near the 3D limit to gapped in the quasi-1D regime.

10:24AM V3.00005 A Three-Component Degenerate Fermi Gas. SEILIM JOCHIM, Max-Planck-Institute for Nuclear Physics and Heidelberg University — We have realized a three-component Fermi gas consisting of the three lowest spin states (|1⟩, |2⟩, |3⟩) of the Li atom. Interactions in this system are governed by three different scattering lengths (a_{12}, a_{23}, a_{13}) between the three states, which all exhibit broad and overlapping Feshbach resonances. This enables us to tune the interactions of the system to become both strongly repulsive and strongly attractive, making it a generic three-component system. It is therefore ideally suited to study predictions of exotic phases such as color superconductivity that are expected for example inside of neutron stars. It is also possible to tune the scattering lengths to very small values simultaneously, which facilitates the preparation of the mixture: Starting from a degenerate mixture of atoms in states |1⟩ and |2⟩, we simultaneously apply radio frequencies resonant with the |1⟩-|2⟩ and |2⟩-|3⟩ transitions. This causes the three states to be mixed. To obtain an incoherently mixed sample within a few hundred milliseconds we apply a small magnetic field gradient along the weak axis of our trap. In first experiments we studied the collisional stability of our gas with respect to the magnetic field |1⟩. We observe an intriguing three-body loss resonance that occurs when all two-body scattering lengths are negative and no two-body bound state exists. The mixture is stable where the scattering lengths are relatively small, which is an important prerequisite for the preparation of the gas. The stable gas is also a good starting point for experiments in the strongly interacting regime, where we aim to observe many-body effects. Progress on this effort will be reported.

References:

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V4 DPOLY DCMP: Microgels: Colloidal Properties of Gels 306/307

8:00AM V4.00001 Melting and Frustration in Temperature-Sensitive Colloids1. ARJUN YODHI, University of Pennsylvania — I will review experiments from my laboratory that employ temperature-sensitive microgel particles to induce novel phase behavior in suspension. This phenomenon offers a fantastic new variable for control of lyotropic suspensions. Recent experiments, for example, have enabled us to learn how three-dimensional crystals first begin to melt [1], to directly observe melting in 2-D wherein intermediate hexatic phases form [2], and to create geometrically frustrated colloidal “anti-ferromagnets” [3].

References:

1This work was supported by the NSF through grants DMR-0520020 (MRSEC), DMR-080488 and by NASA, through grant NAG-2939.

8:36AM V4.00002 Equilibrium features in the arrested phase separation of PNiPAM microgels, VERONIQUE TRAPPE, Dept. of Physics, University of Fribourg, Switzerland — We investigate the arrested phase separation of poly-N-isopropylacrylamide (PNiPAM) microgels. At large enough concentrations we observe the formation of a macroscopic gel-body that exhibits a peculiar temperature dependence. In a temperature-range, where the volume of the individual particles no longer changes, the final dimension of the macroscopic gel body depends on the depth of the quench into the phase separation regime. Increasing the quench depth results in a decrease of the dimension of the gel-body; this is reminiscent of a thermodynamically driven phenomenon and contrasts with the fact that the formation of the gel-bodies is due to the arrest of a phase separation process.
modeling and experiments has greatly accelerated our efforts, and several examples illustrating the benefits of this approach will be presented. An overview of recent efforts at Ford aimed at developing new materials for reversible, solid state hydrogen storage. A tight coupling between first-principles efficient storage of hydrogen has been identified as one of the key materials-based challenges to realizing a transition to FC vehicles. This talk will present fossil-fuel-powered internal combustion engines – namely, the proton exchange membrane FC – utilizes hydrogen as a fuel. Although hydrogen has about three

References:


This work was done in collaboration with Liquan Pei and John R. Savage. We gratefully acknowledge support from Research Corporation and from the NSF through grant DMR-0605839.

10:24AM V4.00005 Phase behavior and rheology of ionic microgels, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Our aim is to understand and control the mechanical properties of dense microgel suspensions, where the softness of the constituent particles can have important effects over the macroscopic behavior. In particular, we are using ionic microgel particles based on poly(vinylpyridine), a monomer that ionizes with pH. When de-swollen, the particles are essentially charged hard spheres and crystallize at high enough volume fractions. By contrast, when the microgels are swollen, light and neutron scattering experiments show that the suspension does not crystallize, irrespective of particle density. But even more remarkably, these highly packed systems remain essentially liquid and do not seem to exhibit glassy behavior. This phenomenology is markedly different to that of ordinary colloids and suggests that the properties of the single particle can dramatically affect the phase behavior and mechanical properties of the packed suspension.

Thursday, March 19, 2009 8:00AM - 11:00AM – Session V5 FIAP: Computational Design of Hydrogen Storage Materials 401/402

8:00AM V5.00001 Computational Discovery of Novel Hydrogen Storage Materials and Reactions, CHRISTOPHER WOLVERTON, Northwestern University — Practical hydrogen storage for mobile applications requires materials that exhibit high hydrogen densities, low decomposition temperatures, and fast kinetics for absorption and desorption. Unfortunately, no reversible materials are currently known that possess all of these attributes. Here we present an overview of our recent efforts aimed at developing a first-principles computational approach to the discovery of novel hydrogen storage materials. We have developed computational tools which enable accurate prediction of decomposition thermodynamics, crystal structures for unknown hydrides, and thermodynamically preferred decomposition pathways. We present examples that illustrate each of these three capabilities. Specifically, we focus on recent work on crystal structure and dehydriding reactions of borohydride materials, such as Mg(BH₄)₂, MgB₆H₁₂, and mixtures of complex hydrides such as the ternary LiBH₄/LiNH₄/MgH₂ system. References:


8:36AM V5.00002 Combining computation and experiment to accelerate the discovery of new hydrogen storage materials, DONALD SIEGEL, Ford Motor Company — The potential of emerging technologies such as fuel cells (FCs) and photovoltaics for environmentally-benign power generation has sparked renewed interest in the development of novel materials for high density energy storage. For applications in the transportation sector, the demands placed upon energy storage media are especially stringent, as a potential replacement for fossil-fuel-powered internal combustion engines – namely, the proton exchange membrane FC – utilizes hydrogen as a fuel. Although hydrogen has about three times the energy density of gasoline by weight, its volumetric energy density (even at 700 bar) is roughly a factor of six smaller. Consequently, the safe and efficient storage of hydrogen has been identified as one of the key materials-based challenges to realizing a transition to FC vehicles. This talk will present an overview of recent efforts at Ford aimed at developing new materials for reversible, solid state hydrogen storage. A tight coupling between first-principles modeling and experiments has greatly accelerated our efforts, and several examples illustrating the benefits of this approach will be presented.
9:12AM V5.00003 Novel hydrogen storage approaches using organometallics, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — Storing molecular hydrogen in organometallics can ensure fast kinetics, low heat management, high energy efficiency, and superb reversibility. The gravimetric density is, however, low for room temperature storage. The reason for the too low density is because the binding is too weak. First-principles calculations [1,2] suggested that organometallics may significantly increase the binding, which is also correlated with decreasing inter-molecular distances and hence a significantly increased volumetric density [3]. Current experimental difficulties are twofold: a) how to synthesize the organometallics and b) how to avoid the transition metal atoms from clustering [4]? Recent experiment [5] on titanium-doped porous silica and theoretical predictions on calcium doping [3,6] may shed new lights on these difficult problems.


9:48AM V5.00004 Computational methods to determine the structure of hydrogen storage materials², TIM MUELLER, Massachusetts Institute of Technology — To understand the mechanisms and thermodynamics of material-based hydrogen storage, it is important to know the structure of the material and the positions of the hydrogen atoms within the material. Because hydrogen can be difficult to resolve experimentally, computational research has proven to be a valuable tool to address these problems. We discuss different computational methods for identifying the structure of hydrogen storage materials and the positions of hydrogen atoms, and we illustrate the methods with specific examples. Through the use of ab-initio molecular dynamics, we identify molecular hydrogen binding sites in the metal-organic framework commonly known as MOF-5 [1]. We present a method to identify the positions of atomic hydrogen in imide structures using a novel type of effective Hamiltonian. We apply this new method to lithium imide (Li2NH), a potentially important hydrogen storage material, and demonstrate that it predicts a new ground state structure [2]. We also present the results of a recent computational study of the room-temperature structure of lithium imide in which we suggest a new structure that reconciles the differences between previous experimental and theoretical studies.

²Supported by the U.S. Department of Energy grant DE-FG02-05ER46253.

10:24AM V5.00005 Kinetics of bulk and surface mass transport in complex metal hydrides, HAKAN GUNAYDIN, UCLA — Metal hydrides can be used to store hydrogen in high gravimetric and volumetric densities. However, the kinetics of hydrogen release and uptake are slow in complex metal hydrides. Clarification of the mechanism of hydrogen release and uptake in complex metal hydrides can aid in a rational design of new hydrogen storage materials with fast kinetics or catalysts that will catalyze the rate of hydrogen release from the existing materials. The release of hydrogen in metal hydrides requires the transport of hydrogen and/or heavier species. The kinetics of such mass transport in metal hydrides can be the rate-limiting process for the release of hydrogen. For example, the rate-determining step for the release of hydrogen from NaAlH4 is the creation and diffusion of neutral AlH3 defects in NaAlH4. The release of hydrogen from LiH destabilized LiNH2 also proceeds via the creation of neutral point defects. The mechanism of mass transport in prototypical hydrogen storage materials such as NaAlH4 and LiNH2 and the mechanism of hydrogen diffusion in aluminum will be discussed.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V6 DCOMP: Recent Advances in Biomolecular Simulations 406

8:00AM V6.00001 Metadynamics simulation of large scale motion in proteins, MICHELE PARRINELLO, Department of Chemistry and Applied Biosciences, ETH Zurich, USI Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland — Understanding large scale protein motions is essential in the study of many biological processes. Molecular dynamics simulations could provide important clues, but they are hampered by the fact, that they can only explore time scales, smaller than most interesting phenomena. To circumvent this problem, our group has developed a number of enhanced sampling techniques that allow exploring many such long time scale phenomena. In particular, a very recent development permits reconstructing complex pathways without the need of introducing collective variable. A number of large scale applications will be presented.

8:36AM V6.00002 Quantum Simulations of Solvated Biomolecules Using Hybrid Methods, MIROSLAV HODAK, North Carolina State University — One of the most important challenges in quantum simulations on biomolecules is efficient and accurate inclusion of the solvent, because the solvent atoms usually outnumber those in the biomolecule of interest. We have developed a hybrid method that allows for explicit quantum-mechanical treatment of the solvent at low computational cost. In this method, Kohn-Sham (KS) density functional theory (DFT) is combined with an orbital-free (OF) DFT. Kohn-Sham (KS) DFT is used to describe the biomolecule and its first solvation shells, while the orbital-free (OF) DFT is employed for the rest of the solvent. The OF part is fully O(N) and capable of handling 10⁵ solvent molecules on current parallel supercomputers, while taking only ~ 10 % of the total time. The compatibility between the KS and OF DFT methods enables seamless integration between the two. In particular, the flow of solvent molecules across the KS/OF interface is allowed and the total energy is conserved. As the first large-scale applications, the hybrid method has been used to investigate the binding of copper ions to proteins involved in prion (PrP) and Parkinson’s diseases. Our results for the PrP, which causes mad cow disease when misfolded, resolve a contradiction found in experiments, in which a stronger binding mode is replaced by a weaker one when concentration of copper ions is increased, and show how it can act as a copper buffer. Furthermore, incorporation of copper stabilizes the structure of the full-length PrP, suggesting its protective role in prion diseases. For alpha-synuclein, a Parkinson’s disease (PD) protein, we show that Cu binding modifies the protein structurally, making it more susceptible to misfolding — an initial step in the onset of PD. In collaboration with W. Lu, F. Rose and J. Bernholc.
9:12AM V6.00003 Urea’s action on the hydrophobic interaction in physical and biophysical systems

B.J. BERNE, Columbia University — For more than a century, urea has been commonly used as an agent for denaturing proteins. However, the mechanism behind its denaturing power is still not well understood. The mechanism of denaturation of proteins by urea is explored using all-atom molecular dynamics simulations of hen lysozyme generated on BlueGene/L. Accumulation of urea around lysozyme shows that water molecules are expelled from the first hydration shell of the protein. We observe a two stage penetration of the protein, with urea penetrating the hydrophobic core before water, forming a “dry globule.” The direct dispersion interaction between urea and the protein backbone and sidechains is stronger than for water, which gives rise to the intrusion of urea into the protein interior and also to urea’s preferential binding to all regions of the protein. This is augmented by preferential hydrogen bond formation between the urea carbonyl and the backbone amides which contributes to the breaking of intra-backbone hydrogen bonds. Our study supports the “direct interaction mechanism” whereby urea has a stronger dispersion interaction with protein than water. We also show by molecular dynamics simulations that a 7 M aqueous urea solution unfolds a chain of purely hydrophobic groups which otherwise adopts a compact structure in pure water. The unfolding process arises due to a weakening of hydrophobic interactions between the polymer groups. Again the action of urea is found to be direct, through its preferential binding to the polymer or plates. It is, therefore, acting like a surfactant capable of forming hydrogen bonds with the solvent. The preferential binding and the consequent weakened hydrophobic interactions are driven by enthalpy and are related to the difference in the strength of the attractive dispersion interactions of urea and water with the polymer chain or plate. We also show that the indirect mechanism, in which urea acts as a chaotrope, is not a likely cause of urea’s action as a denaturant. These findings suggest that, in denaturing proteins, urea (and perhaps other denaturants) forms stronger attractive dispersion interactions with the protein side chains and backbone than does water and, therefore, is able to dissolve the core hydrophobic region.

9:48AM V6.00004 Systematic Coarse-Graining of Biomolecular Systems

GREG VOTH, University of Utah — A multiscale theoretical and computational methodology will be presented for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the methodology is the multiscale coarse-graining method for rigorously deriving coarse-grained models from the underlying molecular-scale forces. Applications of the multiscale approach will be given for membranes and proteins. Recent advances in coarse-graining large protein complexes will also be described along with key applications.

10:24AM V6.00005 Multi-resolution protein modeling by combining theory and experiment

CECILIA CLEMENTI, Rice University — The detailed characterization of the overall free energy landscape associated with the folding process of a protein is the ultimate goal in protein folding studies. Modern experimental techniques provide accurate thermodynamic and kinetic measurements on restricted regions of a protein landscape. Although simplified protein models can access larger regions of the landscape, they are oftentimes built on assumptions and approximations that affect the accuracy of the results. We present new methodologies that allows to combine the complementary strengths of theory and experiment for a more complete characterization of a protein folding landscape at multiple resolutions. Recent results and possible applications will be discussed.

Thursday, March 19, 2009 8:00AM - 10:24AM
Session V7 GMAG: Applications of Magnetic Thin Films with Tilted Anisotropy

8:00AM V7.00001 Magnetic Thin Films for Perpendicular Recording

KAI-ZHONG GAO, Seagate Technology — Magnetic recording technology has shown a rapid growth over the past decade or more with the areal density growth rate more than 40% due to introduction of giant magneto-resistive (GMR), tunneling magneto-resistive (TMR) head and perpendicular recording technology. Current products are in the range of 300-400Gb/in² and demonstrations of 600-800Gb/in² have occurred for perpendicular recording. Recent progresses are mainly due to improvement in magnetic thin film media signal to noise ratio. In this talk, we give a brief summary of recent progresses on perpendicular recording media technology and look at possible extension for ultra high areal density recording based on recording physics and media designs. First we are going to give a brief review on the advantages of the 1st generation of perpendicular recording media as compared to longitudinal recording media. Then the effect of media switching field and switching field distribution will be discussed. We show several different media designs and show its impact to the recording technology, including media with tilted anisotropy, media with coupled granular continuous (CGC) structure, media with exchange coupled composite structure and media with exchange spring system. In addition, we will discuss the impact of media grain size on achievable areal density, the ultimate limit for magnetic recording based on continuous media. Finally, a possible extension and its impact are discussed. As stated before, here we will not try to dig into very specific detail of each topic but look at the basic concept and physics behind each topic that may potentially lead to new technology break through.

8:36AM V7.00002 Approaches and Applications of Tilted Magnetic Anisotropy in Hard Disk and STT-RAM Magnetic Recording for Extremely High Areal Density

JIAN-PING WANG, University of Minnesota — Using tilted magnetic anisotropy in magnetic recording media has been proposed and demonstrated to address several key challenges for future hard disk magnetic recording several years ago. Recent simulations show the potential benefit of using tilted magnetic anisotropy in patterned composite magnetic media that can supports the recording areal density up to several Terabit per square inch. In this talk, I will first present the fundamental physics of the advantages of using tilted magnetic anisotropy in magnetic recording media and spin torque transfer random access memory (STT-RAM). Then several approaches to experimentally make magnetic films in tilted anisotropy media will be presented and discussed in details. These include: 1) crystallographically controlling the tilted magnetic easy axis by using proper underlayers and seedlayers; 2) physically engineering the tilted magnetic easy axis by oblique sputtering on smooth or curved substrates; 3) mechanically engineering the tilted magnetic easy axis by self-assembling magnetic nanoparticles with special shape (such as octahedral-shaped L10 phase FePt nanoparticles); 4) micromagnetically engineering the tilted magnetic easy axis by exchange-coupling two magnetic layers with different magnetic easy axis and anisotropy constant. Results based on hcp phase Co-alloy and L10 phase FePt and FePd films will be presented in details. Finally, I will propose and discuss how to use tilted magnetic anisotropy for the magnetic free layer in the magnetic tunnel junction (MTJ) to reduce the critical switching current density while keeping the thermal stability, which can extend the recording density of the proposed STT RAM further.

The author thanks the support from Information Storage Industry Consortium (INSIC) Extremely High Density Recording Program (EHDR), NSF ECCS 0702264 and NSF Minnesota MRSEC.
9:12 AM V7.00003 Magnetic nanocap arrays with tilted magnetization. MANFRED ALBRECHT, Chemnitz University of Technology — In modern magnetic recording materials the "superparamagnetic effect" has become increasingly important as new magnetic hard disk drive products are designed for higher storage densities. In this regard, patterned media [1], where two-dimensional arrays of nanostructures are used, is one of the concepts that might provide the required areal density in future magnetic recording devices. However, also nanostructure arrays will ultimately need high anisotropy material such as L10-FePt to provide enough thermal stability and thus much higher writing fields than currently obtainable from perpendicular magnetic recording heads. One proposed solution to this problem is the use of tilted magnetic recording media [2]. The basic idea is to tilt the easy axis of the magnetic medium from the perpendicular direction by 45 degrees. In this case, the switching field will be reduced by a factor of two in the Stoner-Wohlfarth limit. Recently, this approach was realized by oblique film deposition onto arrays of self-assembled spherical particles [3-5]. In this presentation, recent results on different film systems including Co/Pt multilayers, FePt and CoPtCr-SiO2 alloys which have been deposited onto SiO2 particle monolayers will be presented. It turned out that by tuning the growth conditions single domain nanocaps with enhanced magnetic coercivity and tilted anisotropy axis can be achieved even for particle sizes below 50 nm.

References

9:48 AM V7.00004 Spin-torque oscillators with tilted fixed layer magnetization. CHAOLIN ZHA, Department of Microelectronics and Applied Physics, Royal Institute of Technology, Sweden — One of the promising applications based on the spin transfer effect [1-3] is the Spin Torque Oscillator (STO) with signal generation at microwave frequencies related to ferromagnetic resonance. The STO may be thought of as a nanoscopic Yttrium Iron Garnet (YIG) oscillator with a similarly broad frequency range, but significant advantages such as easy on-chip integration, and current tunability instead of only field tunability. However, STOs still typically require a large, static, magnetic field for operation; removing the need for this field is currently an intensely researched topic. Three different STO designs have been attempted to address zero field operation: i) the perpendicularly polarized STO [4], ii) the wavy torque STO [5], and iii) the vortex STO [6]. Recently we proposed the Tilted Polarizer STO (TP-STO) having a fixed layer with an out-of-plane magnetic easy-axis tilted a finite angle away from the film normal [7]. In this talk, I will review our simulation work of the TP-STO and show its potential to generate large output signal in zero field. I will present detailed structural and magnetic characterization of single layer L10 (111) FePt with tilted magnetic anisotropy and show how we have fabricated FePt/Cu/NiFe pseudo spin valves with magnetoresistance values of about 0.5%, and as much as 5% if each interface is doped with CoFe. Finally, I will present our preliminary work on observing actual microwave signal generation in nano-contact TP-STOs and discuss their potential for applications.

References

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V8 FPS DBP: The Physics of Imaging and Radiotherapy 414/415

8:00 AM V8.00001 Dedicated breast CT. JOHN BOONE, University of California Davis — Dedicated breast computed tomography (CT) systems were designed and fabricated in our laboratory, and patient scanning commenced in November 2004. The breast CT scanner was designed utilizing several off-the-shelf components, including the x-ray system, the flat-panel detector, and a position encoder - bearing - motor system. These components were integrated into a custom designed scanner frame and gantry. The breast CT scanners utilize a 17 second acquisition during patient breath-hold, and during this time 500 projection images are acquired over 360 degrees around the breast. The radiation levels are adjusted such that the mean glandular dose is equal to that of traditional diagnostic imaging, robotically controlled biopsy, and other interventional procedures.

8:36 AM V8.00002 Tomographic Imaging: Visualization of the Unseeable. XIAOCHUAN PAN, The University of Chicago — Tomographic imaging is a noninvasive approach to acquiring information within the subject under study, and it plays an increasingly important role in the improvement of health care by providing valuable information for diagnosis of diseases, for guidance of disease treatment and therapy, and for assessment/monitoring of treatment response. It has also found a wide variety of applications in other disciplines, ranging from molecular imaging to material sciences to security scan to paleontology. Over the last 30 years, biomedical imaging has involved into an important discipline in its own right. Physics and mathematics form the foundation of advanced tomographic imaging. Computed tomography (CT) and magnetic resonance imaging (MRI) represent two well-known tomographic imaging modalities. In this talk, I will first introduce the basic physics and mathematics principles on which some of the advanced tomographic imaging techniques such as CT are based, with an emphasis on what and how physical signals are detected, how they are used for producing images, and what physical information is that can be extracted from these images. I will then touch upon some of the recent exciting advances in tomographic imaging technology, followed by a brief discussion of some of the important applications of advanced tomographic imaging in medicine and other areas.

References

3Department of Radiology, Department of Radiation and Cellular Oncology, The College, Committee on Medical Physics, and Cancer Research Center, The University of Chicago

9:12 AM V8.00003 Planning and Delivery of Radiation TherapyPrinciples and Recent Developments. CEDRIC YU, University of Maryland School of Medicine — No abstract available.
states for different system sizes. In contrast to earlier studies, the average connectivity ("degree") of each agent is constant here, independent of the system sharing the same opinion and with opponents. Using simulations and analytic arguments, we determine the final steady states and the relaxation into these addition, we incorporate the rapidly changing nature of the interpersonal relations in the model. At each time step, agents can update their relationships, so system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In ABHISHEK MUKHOPADHYAY, BEATE SCHMITTMANN, Physics Department, Virginia Tech — We study a simple model for voter dynamics in a two-party system. The opinion formation process is implemented in a random network of agents in which interactions are not restricted by geographical distance. In
9:24AM V9.00008 Dynamics of priority-queue networks, BYUNGJOON MIN, KWANG-IL GOH, IN-MOOK KIM, Korea University — Recent application of priority queue models for human dynamics opened a way to study the human behavior under quantiative framework. Given the evident active engagement in social networking of individuals, dynamics of priority queues forming networks needs to be understood. Along this line, here we study the dynamics of priority-queue networks by generalizing the binary interacting priority queue model of Oliveira and Vazquez (OV). We found that the OV model with AND-type protocol for interacting tasks is in general not scalable for the queue networks with more than two queues, because the dynamics for interacting tasks become highly correlated. We thus propose a model with OR-protocol. Of further interest is to explore the effects of the number of queues and the network topology on the waiting time dynamics of the priority-queue networks, finding that its distribution exhibits power-law tail in all cases considered, yet with exponents dependent on the network topology. We also show that when the tasks in the queue networks are executed synchronously, priority conflicts affect the waiting time dynamics strongly, resulting in a different power law.

9:36AM V9.00009 About human activity, long-term memory, and Gibrat’s law1, DIEGO RYBSKI, Levich Institute, City College of New York, New York, NY 10031, SERGYEV. BULDYREV, SHLOMO HAVLIN, FREDRIK LILJEROSS, HERMAN A. MAKSE — A central research question in the social sciences for several centuries has been whether any law like patterns in the unintended outcomes of human action exist. Here we investigate the existence of scaling laws in the human activity of communication, considering the number of messages sent by individuals as a growth process in time. We analyze millions of messages sent in two social online communities and uncover power-law relations between fluctuations in the growth rate and the activity of the members. We attribute this scaling law to a long-term persistence of human activity beyond daily or weekly cycles holding up to more than a year. Based on such an underlying long-term correlated dynamics, we elaborate a consistent framework for the empirical evidences, establishing a missing link between the scaling behavior in the growth and long-term persistence. Our results indicate that large fluctuations in communication activity can be expected as an unintended consequence of human interaction. This finding is of importance for both designing communication systems and for understanding the dynamics of social systems.

1NSF-HSD

9:48AM V9.00010 Tour de Sys: The traveler’s view of a network, DANIEL GRADY, CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University, Evanston IL, USA — The plight of the Flattander is imperfect information about a high-dimensional object. Yet even so, the clever inhabitant of a low-dimensional world can gain a great deal of information about such an object by examining it from many perspectives. We analyze complex transportation networks by using shortest-path trees to measure universal network properties from different locations. Furthermore, by defining a measure of a node’s geographical access area we give a more realistic characterization of the centrality or remoteness of a location. The network topology indicates a clear distinction between the center and edge of a network, but we find that examining the weights of links is crucial, as the distinction in the weighted network for some quantities is even more pronounced. Often prior research has not focused on the weightedness of transportation networks, in spite of the fact that this property has an obvious bearing on how the networks are actually used. We show that measuring networks with weighted edges significantly affects their statistics. Our analysis indicates dynamical processes occurring on these networks should behave in a manner very different than what is predicted by considering topology alone.

10:00AM V9.00011 Universality and the lack of it in multiscale human mobility networks, RAFAEL BRUNE, CHRISTIAN THIEMANN, DIRK BROCKMANN, Northwestern University, Evanston, IL, USA — Although significant research effort is currently devoted to the understanding of complex human mobility and transportation networks, their statistical features are still poorly understood. Specifically, to what extent geographical scales impose structure on these networks is largely unknown. In particular, in light of the use of human mobility models in the development and testing theories for spatial disease dynamics, a comprehensive understanding of their structure is of fundamental importance. The large majority of statistical properties (degree distributions, centrality measures, clustering, etc.) of these networks have been obtained either for large scale networks or on small scale systems, indicating significant yet poorly understood deviations. We will present the first investigation of multiscale and multi-national mobility networks, covering length scales of a few to a few thousand kilometers. We will report that certain properties such as mobility flux distribution are universal and independent of length scale, whereas others vary systematically with scale. In particular, controversial properties such as scale-free degree distributions lose their heavy tails in small to intermediate length-scale windows.

10:12AM V9.00012 Monte Carlo Studies of the Isoperimetric Dimension of Growing Droplets in Metastable Decay of the Ising Model on Small-World Graphs, HOWARD L. RICHARDS, Physics & Physical Science, Marshall University — For the Ising model on a regular, nearest-neighbor lattice of less than 6 dimensions, metastable decay occurs via the nucleation of critical droplets: subcritical droplets are biased toward shrinkage, whereas supercritical droplets are biased toward growth. The size of a critical droplet is governed by the competition between the coupling of the magnetic field to the volume of the droplet, which lowers the free energy, and the coupling of the droplet of the stable state to metastable state at the boundary of the droplet, which increases the free energy. This competition between volume effects and surface effects makes the isoperimetric dimension relevant to metastable decay. The simulations discussed here are for a triangular lattice with a small percentage of “small-world” connections. The system initially has only one “down” spin, from which the droplet grows; switching is irreversible and only occurs for “up” spins adjacent to at least one “down” spin.

10:24AM V9.00013 Functional vs. Structural Modularity: do they imply each other?1, ZOLTAN TOROCZKAI, University of Notre Dame — While many deterministic and stochastic processes have been proposed to produce heterogeneous graphs mimicking real-world networks, only a handful of studies attempt to connect structure and dynamics with the function(s) performed by the network. In this talk I will present an approach built on the premise that structure, dynamics, and their observed heterogeneity, are implementations of various functions and their compositions. After a brief review of real-world networks where this connection can explicitly be made, I will focus on biological networks. Biological networks are known to possess functionally relevant features in addition to obvious structural ones. While proposals have been made for the evolutionary emergence of modularity, it is far from clear that adaptation on evolutionary timescales is the sole mechanism leading to functional specialization. We show that non-evolutionary learning can also lead to the formation of functionally specialized modules in a system exposed to multiple environmental constraints. A natural example suggesting that this is possible is the cerebral cortex, where there are clearly delineated functional areas in spite of the largely uniform anatomical construction of the cortical tissue. However, as numerous experiments show, when damaged, regions specialized for a certain function can be retrained to perform functions normally attributed to other regions. We use the paradigm of neural networks to represent a multitasking system, and use several non-evolutionary learning algorithms as mechanisms for phenotypic adaptation. We show that for a network learning to perform multiple tasks, the degree of independence between the tasks dictates the degree of functional specialization emerging in the network. To uncover the functional modules, we introduce a method of node knockouts that explicitly rates the contribution of each node to different tasks (differential robustness). Through a concrete example we also demonstrate the potential inability of purely topology-based clustering methods to detect functional modules. The robustness of these results suggests that similar mechanisms might be responsible for the emergence of functional specialization in other multitasking networks, as well, including social networks.

1Co-Authors: Sameet Sreenivasan (U. Texas Austin) and Hyunjoo Kim (U. Notre Dame)

Thursday, March 19, 2009 8:00AM - 10:48AM
Session V10 DCMP: Artificially Structured Materials for Optical Manipulation 304
discuss the possibility of generating and detecting these waves in porous metals and porous superconductors. We have also calculated the plasmonic band structure for waves propagating through a three-dimensional inverse opal structure of pores in a metallic host. In contrast to the analogous plasmonic waves propagating along periodic chains of metallic nanoparticles in a dielectric, the pore waves do not suffer radiative losses, and the tight-binding approach is not restricted to the quasistatic approximation or to particles small compared to a wavelength. We dispersion relations and group velocities of plasmonic waves propagating along a periodic chain of nanoscale pores in a Drude metal, using a tight-binding approach to provide in-plane measurements of the strength of the scatter in all transmitted and reflected angles. This data is used to generate Bi-directional Scatter Distribution Functions (BSDFs), which can be either physically or empirically based, to model the reflected and transmitted scatter for all incident angles.

8:36AM V10.00004 ABSTRACT WITHDRAWN —

8:48AM V10.00005 Theory of Plasmonic Wave Propagation Along a Periodic Chain of Nanoscale Pores in a Metal, DAVID STROUD, Ohio State Univ., KWANGMOO KIM, Univ. of Maryland — We have calculated the dispersion relations and group velocities of plasmonic waves propagating along a periodic chain of nanoscale pores in a Drude metal, using a tight-binding approach. The propagating modes are Bloch waves constructed from linear combinations of electromagnetic modes of the individual pores embedded in a metallic host. In contrast to the analogous plasmonic waves propagating along periodic chains of metallic nanoparticles in a dielectric, the pore waves do not suffer radiative losses, and the tight-binding approach is not restricted to the quasistatic approximation or to particles small compared to a wavelength. We have also calculated the plasmonic band structure for waves propagating through a three-dimensional inverse opal structure of pores in a metallic host.

We discuss the possibility of generating and detecting these waves in porous metals and porous superconductors.

1Supported by NSF Grant DMR04-13395 (DS) and MRSEC Grant DMR05-20471 (KK)
9:48AM V10.00010 Transformation media with negative refractive indices1, C.T. CHAN, Physics, HKUST, Hong Kong, Y. LAI, H.Y. CHEN, JACK NG, Z.Q. ZHANG, PHYSICS DEPARTMENT, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY, HONG KONG TEAM — Artificially structured materials with a negative refractive index designed by transformation optics can have interesting properties. Based on merging the concept of complementary media and transformation media, we propose an invisibility cloak operating at a finite frequency that can make an object invisible with a pre-specified shape and size within a certain distance outside the shell. The cloak is comprised of a dielectric core, a negative index metamaterial shell and an “anti-object” embedded inside the shell. The cloaked object is not blinded by the cloaking shell since it lies outside the cloak. Full-wave simulations in two dimensions have been performed to verify the cloaking effect. We also show that a positive index core coated with a negative index shell can result in a frequency selective super-absorber which has an absorption cross section that is significantly higher than the geometric cross section.

1Supported by HK RGC

10:00AM V10.00011 Electromagnetic transparency by graded metallic coating2, L. SUN, K.W. YU, The Chinese University of Hong Kong — Recently there has been an increasing interest in achieving cloaking or invisible devices for electromagnetic fields. The study has been based on Pendry’s transformation media concept. In this work, we have studied electromagnetic scattering by coated spheres with a homogeneous core and a radially inhomogeneous dielectric shell described by the lossless graded Drude model \( \varepsilon(r) = 1 - \omega_p^2(r)/\omega^2 \). The plasma frequency depends on \( r \) as \( \omega_p^2 = 1 - cr^2 \), where \( c \) and \( k \) are positive constants. The electromagnetic field distribution has been calculated within the fully electromagnetic Mie scattering theory. When \( k = 2 \), exact analytic solutions can be obtained for the field distribution in terms of Whittaker functions. The total scattering cross section can be obtained from the scattering field amplitudes and is found to be dependent on both the graded profile and the cross-shell ratio. The analytic expressions of the total scattering cross section allow us to assess the conditions for achieving better transparency[1], resulting in tunable electromagnetic cloaking. [1]. A. Ali and N. Engheta, Phys. Rev. E 72, 016623 (2005)

2Work supported by the General Research Fund of the Hong Kong SAR Government.

10:12AM V10.00012 Wave-Front Engineering by Huygens-Fresnel Principle for Nonlinear Optical Interactions in Domain Engineered Structures1, ZHU YONGYUAN, QIN YIQIANG, ZHANG CHAO, Nanjing University — Wave-front engineering for nonlinear optical interactions was discussed. Using Huygens-Fresnel principle we developed a general theory and technique for domain engineering with conventional quasi-phase-matching (QPM) structures being the special cases. We put forward the concept of local QPM, which suggests that the QPM is fulfilled only locally not globally. Experiments agreed well with the theoretical prediction. The proposed scheme integrates three optical functions: generating, focusing, and beam splitting of second-harmonic wave, thus making the device more compact.

1This work was supported by the State Key Program for Basic Research of China (Grants No. 2004CB619003 and No. 2006CB921804) and the National Natural Science Foundation of China (Grants Nos. 10523001, 10504013, and 10674065).

10:24AM V10.00013 Electromagnetic Response of Josephson Junction Metamaterials in Positive and Negative Permittivity Regimes1, STEVEN ANLAGE, LAURA ADAMS, Center for Nanophysics and Advanced Materials, Physics Department, University of Maryland, College Park, MD 20742-4111 — Negative index of refraction metamaterials have shown strikingly different behavior than their positive index of refraction counterparts, enabling for example cloaking and super lensing. Josephson junction (JJ) metamaterials which are tunable and have low loss are a distinct advantage not only because of their nonlinearity but also due to their ability to be scaled down in size. We will present microwave measurements of JJ arrays that behave differently depending on whether the arrays resonate above or below the cutoff frequency of an electromagnetic waveguide. Below cutoff, resonances indicate a macroscopic phase coherence of the JJ arrays with emission of photons. Above cutoff, we interpret the interaction between the arrays and the electromagnetic waves as indications of vortex-anti-vortex physics. We will describe how the JJ arrays respond to controlled changes of the input power, temperature and dc magnetic fields and how these responses depend on the sign of the permittivity.

1This work was supported by the Intelligence Community Postdoctoral Fellowship program.

10:36AM V10.00014 Anomalous infrared monochromatic transmission through a film of type-II superconductor in magnetic field and a superconducting multiple conductor system, ROMAN YA. KEZERASHVILI, OLEG L. BERMAN, VLADIMIR S. BOYKO, New York City College of Technology, CUNY, YURI E. LOZOVIK, Institute of Spectroscopy — Anomalous far infrared monochromatic transmission through a lattice of Abrikosov vortices in a type-II superconducting film is found. The transmitted frequency corresponds to the photonic mode localized by the defects of the Abrokosov lattice. These defects are formed by extra vortices placed out of the nodes of the ideal Abrokosov lattice. The extra vortices can be pinned by crystal lattice defects of a superconductor. The frequency is studied as a function of magnetic field and temperature in the framework of the Dirac-type two-band model. The control of the transmitted frequency by varying magnetic field and/or temperature is analyzed. Besides, anomalous monochromatic transmission through a superconducting multiple conductor system consisting of parallel superconducting cylinders is found. The transmitted frequency corresponds to the localized photonic mode in the forbidden photonic band, when one superconducting cylinder is removed from the node of the ideal two-dimensional lattice of superconducting cylinders. Our approach is valid for all type-II superconductors but the specific calculations have been performed for the YBCO film in the magnetic field and for the YBCO superconducting cylinders.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V11 DCMP: Transport Phenomena and Electronic Properties of Nanostructures 305

8:00AM V11.00001 Momentum statistics of tunneling electrons in nanoelectromechanical systems, STEVEN D. BENNETT, AASHISH A. CLERK, McGill University — When a mesoscopic conductor is used to measure the position of a nanomechanical oscillator, electrons in the conductor exert a fluctuating back-action force on the oscillator. What is the statistical distribution of the momentum transferred to the oscillator by this force? Motivated by recent experiments that studied a mechanical oscillator coupled to a single tunnel junction[4] or a quantum point contact[5] we investigate theoretically the statistics of back-action force in these systems as well as correlations between the force and the current. Our approach is based on a scattering matrix that depends parametrically on the oscillator position, allowing us to go beyond weak tunneling and study conductors with arbitrary transmittance. We identify two mechanisms of momentum transfer: one involves forces exerted in the scattering region and dominates in the limit of weak tunneling; the other is associated with transferred electron momentum and dominates in the limit of perfect transmission. We also discuss the effects of a spatially asymmetric conductor on the force noise and on the quantum limit of position detection.

5M. Poggio et al., Nat. Phys. 4, 635 (2008).
Mechano-electronic Superlattices in Silicon Nanoribbons

8:12AM V11.00002

Mechano-electronic Superlattices in Silicon Nanoribbons1

M. HUANG, C.S. RITZ, B. NOVAKOVIC, F. FLACK, D.E. SAVAGE, P.G. EVANS, J. KNEZEVIC, University of Wisconsin-Madison, D. YU, Y. ZHANG, F. LIU, University of Utah, M.G. LAGALLY, University of Wisconsin-Madison — Single crystal silicon nanomembranes (SiNMs) have the mechanical compliance fundamentally different from bulk materials or supported thin films that can produce unique structural and electronic effects. The growth of nanostressors on SiNMs utilizes this mechanical compliance to create a “strain lattice” consisting of tiny regions of local curvature in the SiNMs, the order occurring because the locally bending SiNMs provides a strong feedback for self-organization of the nanostressor. We demonstrate that a high degree of order occurs when Ge or SiGe nanostressors are grown on both sides of free-standing but end-tethered Si nanoribbons. Our calculations prove that the strain lattice in the Si produces a modulation in the electronic band structure, and thus an electronic superlattice. Our calculations also demonstrate that discrete minibands can be observable in such an electronic superlattice at 77K. It is expected that an electric conductivity will be increased in the superlattice. We predict that it is possible to observe discrete minibands at room temperature if other nanostressors are used.

1This work was supported by DOE, AFOSR, and NSF.

8:24AM V11.00003

‘Spring-Like’ and Photo-actuated Molecular-Junctions between Nanoparticles

KABEER JASUJA, VIKAS BERRY, Kansas State University — Here we present a study on (1) “molecular-spring” nano-device, where controllable and confined forces are applied on collective molecular-junctions between nanoparticles and (2) photo-actuated nano-junction system where azo-molecules incorporated between nanoparticles apply confined forces to displace them. Both systems are built by using covalently/epitaxially crosslinked polyelectrolyte (cPE) molecules sandwiched between gold nanoparticles (GNP), where cPE molecular-junctions are reversibly compressed and stretched by applying electrically and centrifugally induced forces respectively. The GNPs play a dual role (a) of movable connectors to apply forces and (b) of nanoelectrodes to measure molecular deformation via electron tunneling change. The ‘molecular-spring’ junctions were found to have a spring constant between 10−7 and 10−4 N/m depending on the thickness of the junction. We will also demonstrate the dynamics of these junctions via a motion-in-viscous-media model. The ability to store the compression energy in a molecular-device-architecture and to manipulate these by actuating junctions has the potential to power future molecular devices by stored molecular-energy and controlling properties of nanocomponent based devices.

8:36AM V11.00004

Noise characterization of metal oxide nanowire FETs with electronic properties controlled by surface geometry

WENYONG WANG, University of Wyoming, HAO XIONG, CURT RICHTER, NIST, WOONG-KI HONG, TAKHEE LEE, GIST, NANOWIRE COLLABORATION — In this talk we present the results of low-frequency noise and random telegraph signal (RTS) characterization of metal oxide nanowire (NW) field-effect transistors (FETs). ZnO nanowires with different surface geometry properties such as corrugated and smooth surfaces have been synthesized. FETs fabricated from these NWs exhibit different electronic transport characteristics. Noise characterization has been performed on NW FET devices with different surface properties. The obtained noise power spectra at room temperature show 1/f frequency dependences, and the Hooge’s constants have been calculated from the gate voltage dependence to the 1/f noise for the devices with different surface geometries. The characteristics of low frequency noise in the drain current have been further investigated through random telegraph signals measurements at 4.2 K, where the channel current RTSs can be attributed to the correlated carrier number and mobility fluctuation due to the trapping and detrapping of the carriers by discrete border/surface traps. The effects of the NW surface properties on the RTS behaviors will be discussed.

8:48AM V11.00005

A Bistriator: Modulating the Current of a Nanodevice with a Living Cell

JENNIFER KANE, JASON ONG, RAVI SARAF, University of Nebraska-Lincoln — Isolated single nanoparticles and array of nanoparticles act as a single-electron transistors (SETs) when a single electron is charged. For a typical 5 nm Au particle the switching barrier energy due to Coulomb blockade from a single electron charging is approximately 100 meV, making room temperature switching difficult and very noisy. In an array, the switching energy can be a few eV (at cryogenic temperatures), but unlike a single nanoparticle, the energy barrier reduces linearly and vanishes at room temperature. We have developed a “reactive self-assembly” method to make a network of one-dimensional necklaces of nanoparticles that behaves as a single-electron device at room temperature. Furthermore, upon cementing the particles with an inorganic semiconductor, the switching behavior at room temperature is significantly improved. To demonstrate an interesting application of room temperature single-electron switching, we couple the network to a living microorganism to modulate the device current by regulating the cell’s metabolic activity. In the talk we will describe fabrication of the necklace and biotransistor device.

9:00AM V11.00006

ABSTRACT WITHDRAWN

9:12AM V11.00007

ABSTRACT WITHDRAWN

9:24AM V11.00008

Bistable tunneling current through a quantum dot array junction

YIA-CHUNG CHANG, Research Center for Applied Sciences, Academia Sinica, Taiwan and University of Illinois, Urbana-Champaign, DAVID M.T. KUO, National Central University, Taiwan — We investigate the tunneling current through a six-fold degenerate p–like states of a one- dimensional (1D) or two-dimensional (2D) quantum dot (QD) array in the x-y plane. Due to the coupling of pₓ and pᵧ orbitals at neighboring QDs, a 1D or 2D conduction band (pₓ) is formed, whereas the pᵧ orbitals remain localized due to their weak in-plane coupling. The on-site repulsive Coulomb interaction in the pₓ levels (U) and that between the pₓ level and pₓ/pᵧ level (Uₓₓ) are taken into account in an extended Anderson model, which is used to investigate the tunneling characteristics of the system. Tunneling current through localized pₓ state is calculated in the framework of the Green function technique. Due to the effect of Uₓₓ, the 1D/2D conduction band states are shifted by a self-energy term 2Nuₓₓ. We find that bistable current can be observed for this system in the Coulomb blockade regime, which makes the system a valid candidate for ultra-high-density memory device.

9:36AM V11.00009

Tunneling Between a Quantum Wire and a Two-Dimensional Electron Gas

DOMINIQUE LAROCHE, McGill University and Sandia National Laboratories, JOHN RENO, Sandia National Laboratories, GUILLAUME GERVAIS, McGill University, MIKE LILLY, Sandia National Laboratories — We study 1D-2D tunneling between a quantum wire and a 2D electron gas as a function of magnetic field, source drain bias, temperature and 1D subband occupation. The transition from 2D-2D to 1D-2D tunneling is clearly observed through a sharpening of the tunneling resonance, confirming that the measurements are performed in a 1D-2D state. The device used is fabricated in a GaAs/AlGaAs parallel double quantum well heterostructure with an 11 nm wide Al₀.₉Ga₀.₁As barrier separating the quantum wells. Quantum wires are created via electron beam lithography defined split gates fabricated on both sides of the sample, albeit only one of the wires is used in the experiment. The design is such that the 1D density can be independently controlled over a large conduction range and is uniform over the length of the quantum wire. Both wires show non-ballistic quantum steps up until a conductance of 10 x 2e²/h. Magnetotransport results are compared to tunneling in the 1D-1D and 2D-2D regimes.

1Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract No. DE-AC04-94AL85000.
9:48 AM V11.00010 Temperature Dependence of Electron Tunneling between Quantum Dots and Electron Gas

10:00 AM V11.00011 New insight into Tunneling Process between Quantum Dot and Electron Gas

10:12 AM V11.00012 Hole Transport and Spin Effects in Cleaved-Edge-Overgrowth Quantum Wires

10:24 AM V11.00013 High-quality quantum point contact in two-dimensional GaAs (311)A hole system

10:36 AM V11.00014 ABSTRACT WITHDRAWN

10:48 AM V11.00015 Determination Hanbury-Brown Twiss correlations with electrons and photons

Thursday, March 19, 2009 8:00 AM - 11:00 AM – Session V12 DMP DCMP: Semiconductor Growth and Etching 308

8:00 AM V12.00001 Morphological Study of MBE Grown Iron Nitride Films on Zinc-Blende GaN(001)

— YOKO SAKURAI, SHINTARO NOMURA, YUKIHIRO TAKADA, KENJI SHIRAISHI, University of Tsukuba, MASAKAZU MURAGUCHI, TETSUO ENDOH, Tohoku University, YOKO SAKURAI, SHINTARO NOMURA, YUKIHIRO TAKADA, KENJI SHIRAISHI, University of Tsukuba, MITSUHISA IKEDA, KATSUNORI MAKIHARA, SEIICHI MIYAZAKI, Hiroshima University — We report that gate voltages required for electron injection to quantum dots (QDs) from electron gas and for emission from QDs strongly depend on temperature. For this experiment, Si-QDs floating gate MOS capacitors were designed and fabricated. Displacement current (I) was measured as a function of the gate voltage (V). Peaks in I-V curves appear as a result of charging and discharging of Si-QDs. We have found that the gate voltages for the electron injection to and for the emission from QDs shift toward more positive and negative values with decreasing temperature, respectively. Theoretical study predicts that electron tunneling is strongly enhanced when initial state of 2DES is localized below the QD [1]. Based on this discussion, the experimentally obtained results suggest that localization of electron gas induced by thermal fluctuation is responsible for enhanced electron tunneling.

8:12AM V12.00002 Iron and Iron Nitride Layers on Wurtzite Gallium Nitride Studied Using MBE/STM, WENZHI LIN, JEONGHIM PAK, YINGHAO LIU, KANGKANG WANG, ABHIJIT CHINCHORE, DAVID INGRAM, ARTHUR SMITH, Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, OH 45701, KAI SUN, Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan 48109 — It is of interest to study epitaxial growth of iron and iron nitride (FeN) layers on wurtzite gallium nitride (w-GaN) as a possible magnetic/wide-gap semiconductor system for spintronics. X-ray diffraction (XRD) and reflection high energy electron diffraction (RHEED) of Fe deposited on GaN(0001) suggest the existence of the epitaxial relationship [110]$_{FeN}||[0001]_{GaN}$. Furthermore, multi-streak RHEED patterns indicate the formation of a multi-domain but smooth film. Also, we have investigated the growth of $\sim$1:1 iron nitride on w-GaN(0001) using nitrogen plasma-assisted molecular beam epitaxy (MBE). Both reciprocal and real space techniques were used to study the growth of FeN, including RHEED and scanning tunneling microscopy/spectroscopy (STM/STS). Bulk characterization was also applied, including XRD and transmission electron microscopy (TEM). The results indicate that zinc-blende FeN grows on GaN(0001) with the epitaxial relationship [111]$_{FeN}||[0001]_{GaN}$, and initial atomically-smooth FeN layers are formed. This work has been supported by DOE (Grant #DE-FG02-06ER46317).

8:24AM V12.00003 Stability of Mg-incorporated InN surfaces: first-principles study, T. AKIYAMA, K. NAKAMURA, T. ITO, Mie Univ., Japan, J.-H. SONG, A. J. FREEMAN, Northwestern Univ. — InN films are attractive materials for electronic and optoelectronic applications. The growth of InN epitaxial films with $n$-type and $p$-type conductivity has traditionally been performed along the polar <0001> direction, which may result in large polarization fields along the growth direction, reducing the radiative efficiency of quantum-well light emitters. To overcome this drawback, the growth along nonpolar orientation such as (10$k\bar{2}1$) and (1120) planes and its $p$-type doping have been recently carried out. We have addressed this issue by performing first-principles pseudopotential calculations for Mg-incorporated InN surfaces in various orientations, including (10$k\bar{2}1$) and (1120) as well as (0001) and (0001) surfaces. The calculated surface energies demonstrate that qualitative trends in the stability of Mg-incorporated surfaces agree with those on GaN surfaces, although several surface reconstructions differ from those on GaN surfaces. The effects of growth conditions on $p$-type doping are also discussed.

1 Supported by the NSF’s MRSEC at N. U.

8:36AM V12.00004 Ferromagnetic $\delta - MnGa$ On Wurtzite GaN(0001): Interface Formation And Film Properties, KANGKANG WANG, ABHIJIT CHINCHORE, WENZHI LIN, JEONGHIM PAK, ARTHUR SMITH, Department of Physics and Astronomy, Ohio University, KAI SUN, Department of Materials Science and Engineering, University of Michigan — Ferromagnetic (FM) metal/wide band-gap semiconductor contacts are of great interest due to their potential for novel spintronics applications, such as blue and ultra-violet light-emitting diodes. One promising candidate is $\delta - MnGa$ on wurtzite GaN, whose epitaxial growth has recently been reported, with controllable magnetism via controlling of the Mn:Ga flux ratio. Here we report further studies on MnGa/GaN system grown by N$_2$-plasma equipped molecular beam epitaxy (MBE). Reflection high-energy electron diffraction (RHEED) data suggests a quicker and more abrupt interface formation when grown on Ga-polar GaN surface as compared to N-polar. In-situ scanning tunneling microscopy (STM) measurements on the first few monolayer’s as well as thicker MnGa films will be presented, revealing details of interface formation and other film properties. Stoichiometry dependence of the growth and magnetic properties will also be discussed. This work is supported by DOE (Grant No. DE-FG02-06ER46317) and NSF (Grant No. 0730257). Equipment support from ONR is also acknowledged. [1] S.A. Wolf et al, Science 294, 1488 (2001) [2] E.Lu et al, Phys.Rev.Lett. 97, 146101 (2006)

8:48AM V12.00005 Low-temperature transport properties of disordered tantalum and tantalum nitride films, NICHOLAS BREZNAY, MIHIR TENDULKAR, AHARON KAPITULNIK, Stanford University — Tantalum nitride thin films are used in a wide range of electronic applications, such as in thin film resistors and diffusion barriers in silicon microstructures. Growth and thorough characterization of ultrathin tantalum nitride films may prove useful in potential applications and also facilitate the study of disordered, low-dimensional systems. We will discuss the low-temperature transport properties of reactively sputtered tantalum and tantalum nitride ultrathin films as a function of film structure and composition, and connect our results to recent studies of both these and other similar two-dimensional disordered systems.

9:00AM V12.00006 First Principles Phases of Sub-Monolayer Sr and La on Si (001), KEVIN GARRITY, J.W. REINER, F.J. WALKER, C.H. AHN, S. ISMAIL-BEIJI, Yale, CRISP, CRISP TEAM — The epitaxial integration of complex oxides with semiconductors is a key requirement for many emerging technologies. In the short term, the scaling down of the dielectric layer in current CMOS technology will soon require new materials with higher dielectric constants to prevent quantum mechanical leakage currents. More generally, the epitaxial integration of complex oxides with semiconductors would allow new devices to take advantage of the wide range of oxide properties. To date, the first step of the only known method to grow complex oxides on silicon epitaxially has required 1/2 ML of an alkaline earth metal, usually Sr, to be deposited on a clean silicon surface at about 600 C. Using first-principles density functional theory calculations, we examine the growth of sub-monolayer coverages of both Sr and La on Si (100). For Sr on Si, we report on a novel 1/6 ML structure which explains the complex temperature dependence observed experimentally below 1/2 ML Sr. We compare these results to the case of La on Si, and elucidate some differences which hinder the growth of epitaxial oxides on La template layers. Our results predict an experimentally verified low temperature path to epitaxy using a Sr template layer.

1Supported primarily by NSF MRSEC DMR 0520495.

9:12AM V12.00007 From STM Images to Chemical Understanding: Kinetic Monte Carlo Simulations of Si(100) Etching, ANKUSH GUPTA, IAN T. CLARK, BRANDON S. ALDINGER, MELISSA A. HINES, Cornell University, Ithaca NY — Etching reactions literally write a record of their chemical reactivity in the morphology of the etched surface — a record that can be read using scanning tunneling microscopy (STM) and decoded with the help of simulation. We have developed a fully atomistic kinetic Monte Carlo simulation of Si(100) etching that is appropriate for aqueous etchants that produce fully H-terminated surfaces [e.g., NH$_4$F(aq), KOH(aq) and even H$_2$O]. The model assumes that the reactivity of individual surface sites is determined by the local geometry. As an example, we simulate the production of near-atomically flat Si(100) surfaces, recently observed experimentally, and show that interadsorbate stress plays a crucial role in determining the steady-state etch morphology. The simulated morphologies are in good agreement with experimental observations.
9:24AM V12.00008 Atomic-Scale Effects of Applied Strain on Etching of Si(100). MARC F. FAGGIN, BRANDON S. ALDINGER, ANKUSH GUPTA, MELISSA A. HINES, Cornell University — An ideal hydrogen-terminated Si(100) surface would be highly stressed due to unfavorable steric interactions between neighboring surface sites (i.e. neighboring silicon dihydride species). As a result, some aqueous etchants selectively remove every other silicon dihydride to relieve the stress, producing an unusual striped morphology. In these experiments, we apply a uniaxial strain to the surface during etching. Using a combination of scanning tunneling microscopy and surface infrared spectroscopy, we show that applied strains dramatically alter the etch morphology and the surface species, in some cases promoting the formation of hillocks. These effects are explained in terms of the site-specific reactivity of the etching silicon surface.

9:36AM V12.00009 Aqueous Etching Produces Si(100) Surfaces of Near-atomic Flatness. BRANDON S. ALDINGER, ANKUSH GUPTA, IAN T. CLARK, MELISSA A. HINES, Cornell University — The production of atomically flat Si(100) surfaces is a long-standing technological challenge, as these surfaces are the basis for today’s microelectronic devices. We use a combination of STM and vibrational spectroscopy to show that a simple aqueous etch can produce Si(100) surfaces of surprising and unprecedented smoothness. The etched surfaces are characterized by long rows of H-terminated Si atoms. The chemical origins of this perfection are uncovered, in part, by a new polarization-based, spectral deconvolution technique that significantly simplifies the analysis of the well-known H/Si(100) vibrational spectrum. Kinetic Monte Carlo simulations yield further insights into the site-specific chemical reactions that govern the steady-state etch morphology. The effects of interadsorbate stress, etchant pH, and gas evolution will also be discussed as time permits.

9:48AM V12.00010 Quantitative Correlations of Stress Field and Threading Dislocation Configurations in Si/Si$_{1-x}$Ge$_x$/Si(100) Strained Layers. CHI-CHIN WU, Virginia Military Institute, ROBERT HULL, Rensselaer Polytechnic Institute — The equilibrium configurations of the threading dislocation connecting misfit dislocation dipoles in Si/Si$_{1-x}$Ge$_x$/Si(100) heterostructures have been analyzed by simulation, and compared to experimental images to investigate the correlations of stress field variations and dislocation configuration in capped heteroepitaxial thin films. Calculations are based on the energy equations for dislocations in elastically isotropic crystals over all possible dislocation angular configurations, and the orientations with the minimum total energy are determined as functions of the magnitude and variations of the film stresses. It is determined that the configuration with the misfit dislocation leading at the cap/film interface (as opposed to the film/substrate interface) is increasingly favored either with increasing magnitude of local film stress/strain or with the variation in calculated geometry of the threading dislocation.

10:00AM V12.00011 Ordering mechanisms of periodic stripe arrays on boron-doped Si(100).1 IVAN ERMANOSKI, GARY KELLOGG, NORMAN BARTELT, Sandia National Laboratories — We have used low energy electron microscopy to determine the factors that control the degree of order in as-deposited periodic stripe arrays on the atomically flat Si(100) with high boron doping. The stripes consist of extremely elongated vacancy islands of single atomic height, formed at ∼900°C, confined in micrometer-sized pits. “Perfect” arrays of parallel stripes (in pits of up to ∼10nm in size) were formed by allowing various defects to heal over relatively long periods of time. Sublimation was compensated for by an external Si doser, allowing observation of stripe evolution over the course of hours, with no net loss or gain of Si from the area of interest. Stripe formation and ordering mechanisms include spontaneous nucleation and growth of new islands, longitudinal splitting, as well as coarsening due to surface diffusion. Stripe periodicity depends on temperature, allowing for control of this property. Stripes are stable in a range of ∼100°C, outside of which they assume the familiar shape of elongated islands, shaped by the anisotropy in step energy. Stripe order can be preserved to room temperature by quenching. References: [1] J.-F. Nielsen et al., Appl. Phys. Lett. 79 (2001) 3857

1 Work supported by the U.S. DOE, Office of BES, DMSE. Sandia is operated by Sandia Corporation, a Lockheed Martin Company, for the U.S. DOE’s NNSA under Contract No. DE-AC04-94AL85000.

10:12AM V12.00012 On the Growth Mechanisms of Plasma Deposited Amorphous Silicon Thin Films. DIMITRIOUS MARoudas, SUMEET PANDEY, TEJINDER SINGH, University of Massachusetts, Amherst — We present a theoretical study of the growth mechanism of plasma deposited amorphous silicon (Si) thin films based on kinetic Monte Carlo simulations according to a transition probability database constructed by first-principles density functional theory calculations. Based on the results of the study, we propose a comprehensive mechanism of amorphous Si thin film growth by plasma deposition under conditions that make the silyl radical the dominant deposition precursor. The growth mechanism consists of various surface kinetic events including radical-surface interactions, adsorbed radical-radical interactions, radical surface diffusion, and surface hydride dissociation reactions. Of particular importance to the Si film growth process and the resulting surface composition is the radical dissociative adsorption mediated by Si over-coordination defects along the reaction pathway. The proposed mechanism explains the experimentally measured surface composition of plasma deposited Si films under the deposition conditions considered.

10:24AM V12.00013 Fundamental Study of Boron Carbide Sputtering. SUDARSHAN KARKI, DAE YEOUN, SAAD JANJUA, MARCUS DRIVER, ANTHONY CARUSO, University of Missouri Kansas City — Boron-rich carbides belong to a special class of solids whose main structural unit is the twelve atomicosahedra. When depositing thin films of boron carbide (nominally B$_x$C) by RF or pulsed DC magnetron sputtering, the individual sputtered or ablated cluster size, and the temperature of the substrate to which the clusters adsorb to form the film, greatly affects the bulk film physical and electronic structure. This talk will present mass spectrometry data of the target clusters as a function of RF power, DC bias and chamber pressure toward the goal of modeling and understanding how theicosahedral based boron-rich materials sputter and the resultant control over the final film properties. Argon trapped into the film during the deposition as determined by X-Ray photoemission will also be discussed.

10:36AM V12.00014 Correlation between Bonding Geometry and Band Gap States at Organic–inorganic interfaces: Catechol on Rutile TiO$_2$ (110). ULRlKE DIEBOLD, SHAO-CHUN LI, Department of Physics, Tulane University, JIAN-GUO WANG, Department of Chemistry, Princeton University, PETER JACOBSON, Department of Physics, Tulane University, XUE-QING GONG, ANNABELLA SELLONI, Department of Chemistry, Princeton University — Adsorbate-induced band gap states in semiconductors are of particular interest due to the potential of increased light absorption and photoactivity. A combined theoretical (DFT) and experimental (STM, photoemission) study of the molecular-scale factors involved in the formation of gap states in TiO$_2$ is presented. Using the organic catechol on rutile TiO$_2$ (110) as a model system it is found that the bonding geometry strongly affects the molecular electronic structure. At saturation catechol forms an ordered 4 x 1 overlayer. This structure is attributed to catechol adsorbed on rows of surface Ti$_x$ atoms with the molecular plane tilted from the surface normal by about ±27° in an alternating fashion. In the lowest-energy structure one of the two terminal OH groups at each catechol dissociates and the O binds to a surface Ti atom in a monodentate configuration, while the other OH group forms a H-bond to the next catechol neighbor. Through proton exchange with the surface this structure transforms into one where both OH groups dissociate and the catechol is bound to two surface Ti in a bidentate configuration. Only bidentate catechol introduces states in the band gap of TiO$_2$. 

10:46AM V12.00015 Atomic-Scale Effects of Applied Strain on Etching of Ge(110).1 MARC F. FAGGIN, BRANDON S. ALDINGcr, ANKUSH GUPTA, MELISSA A. HINES, Cornell University — An ideal hydrogen-terminated Ge(110) surface would be highly relaxed due to unfavorable steric interactions between neighboring surface sites (i.e. neighboring silicon dihydride species). As a result, some aqueous etchants selectively remove every other silicon dihydride to relieve the stress, producing an unusual striped morphology. In these experiments, we apply a uniaxial strain to the surface during etching. Using a combination of scanning tunneling microscopy and surface infrared spectroscopy, we show that applied strains dramatically alter the etch morphology and the surface species, in some cases promoting the formation of hillocks. These effects are explained in terms of the site-specific reactivity of the etching silicon surface.
Theoretical adhesion strength of diamond coating with metallic interlayers. 
HAIBO GUO, University of South Carolina, YUE QI, Materials and Processes Lab, GM R&D Center, XIAODONG LI, University of South Carolina — 
Metallic interlayers are often needed to enhance the adhesion of diamond coatings to substrates and to promote diamond nucleation and growth. The interfaces between diamond coatings and metallic interlayer materials with different carbide formation enthalpies, Cu, Al, and Ti, are studied using density functional theory. The ideal interface strength or the work of separation at the interface with the fracture energy of the metal, a fracture is likely to initiate in the metal phase near the interface, therefore a tough metal with a large surface energy is needed to achieve a higher overall toughness. In addition, when the surface energy is larger than the interface energy, a wetted diamond/metal interface is formed during diamond nucleation, which also contributes to good adhesion. The interface energy, which is an energy barrier to diamond nucleation, is found to decrease with the carbide formation enthalpy. These results indicate strong carbide formability and a large surface energy of the interlayer enhances the adhesion and the fracture resistance of the interface, and also conduce to the diamond nucleation on the interlayer.

Thursday, March 19, 2009 8:00AM - 10:36AM —
Session V13 FEd FHP: Physics Education and History

8:00AM V13.00001 Physics Education in Sub-Saharan African Schools and Universities. TILAHUN DERSUSSU, Addis Ababa University — This talk will give an overview of physics teaching and research in Sub-Saharan African Schools and Universities. 
Secondary School Physics Curricula and physics teacher training curricula from 10 African countries are compared from content, methods of delivery and evaluation perspectives. The characteristics of physics study and research in universities, both at the undergraduate and the graduate levels, are described.

8:12AM V13.00002 Physics That Works: Shift in Physics Education Paradigm Based on Work-Integrated Physics Education.1. BAHRAM ROUCHANI, Kettering University — A nontraditional work integrated undergraduate physics degree program that balances the option of pursuing a career path after graduation versus graduate studies will be presented. The main components of this undergraduate physics education model, which will be presented are; work-integrated physics education, emphasis on industrial and applied physics, nontraditional undergraduate research and thesis, an altered academic calendar, required technical sequence courses, and flexibility for each student to engage in courses that best complement physics. The impact on the growth of the physics program, the challenges and rewards involved, as well as pros and cons of such program in contrast with the traditional physics degree programs will be discussed.

1This presentation reflects the work done by the entire Physics Department at Kettering University.

8:24AM V13.00003 Strengthen Instructional Components in Peer-Lead Problem-Solving Workshop with eTEACH. JIA-LING LIN, B. CHOE, P. FOWLER, R. GILSDORF, T. KIRCHDOERFER, A. KOKEMOOR, G. LUCAS, T.J. MAIDEN, A. ROMENS, M. SPRINGER, University of Wisconsin-Madison — Physics and mechanics are core topics that sometimes frighten beginning engineering students. Statistics have shown that an increasing number of students have given up engineering because of struggle in these courses. One common realization is a consensus among educators that the quality of teaching needs to be improved, and that traditional lectures, even with stellar instructors, fail to motivate students to meet learning challenges. One of the responses from the College of Engineering at UW-Madison has been comprehensive academic support services, specifically the Supplementary Instruction (SI) Program. SI, a student-lead problem-solving workshop has made a significant impact on teaching and learning in engineering for the past eight years. In this report, we describe how we develop eTEACH (an on-line teaching tool) to integrate features of subject- and problem-based learning. We discuss how we incorporate eTEACH to promote better interactions between instructors and students, as well as among students. Our initial results showed that this change has assisted students with different learning preferences to improve problem-solving and learning strategies. We acknowledge support from Dr. G. Moses, Dr. D. Woolston, and the 2010 project in engineering college.

8:36AM V13.00004 Student thinking regarding derivative of slope concepts in multivariable calculus1. WARREN CHRISTENSEN, JOHN THOMPSON, University of Maine — Previous work on students’ understanding of graphical interpretation of slope, derivative, and area under curves in various physics contexts has shown substantial difficulties, most notably in kinematics. Concurrently, several reports point toward a lack of algebraic acumen as a likely cause for low achievement in a physics classroom. As part of ongoing research on mathematical challenges that may underlie documented physics difficulties, we focus on single- and multivariable calculus concepts to students near the end of a Calculus III course. Some of the questions are based on our earlier work in thermal physics that are essentially stripped of their physics content. Initial findings show that as many as one in five students encounter some type of difficulty when asked to rank the slopes at five different points along a single path. Students asked to rank the derivatives of three different functions at a single value of the variable face additional difficulties.


8:48AM V13.00005 An Engineer's Physics Lab — using a Large Force Frame. CHRISTY HEID, DONALD RAMPOLLA, Chatham University — We have constructed very economical, easy to assemble force frames that are used by students in our general physics laboratory at Chatham University. The force frame is used at the beginning of the semester to study vector properties of forces. The force frame can be used as a horizontal or vertical force table. Angles of forces are measured using a large movable (rotation and translation) Cartesian coordinate board attached to the frame with large binder clips. The force frame is a versatile device which is used for a number of other experiments, including beam bending and torsion, mechanical resonance, projectile trajectories, torque, mechanical equilibrium, an isolated non-magnetic support for magnetic field experiments, easily adjustable support for inclined plane experiments, support for traveling wave experiments with heavy rope, and support for large scale fluid flow experiments. One advantage to a wood frame is that things can be easily stapled, nailed, screwed or glued just about anywhere on the frame, and damaged frame members can be replaced easily. As one of the few remaining women's undergraduate institutions, we have found the use of these frames to provide an additional advantage in helping women overcome their fear of simple power tools and assembly of mechanical parts as they become comfortable with these through working with the force frames throughout the semester. We intend to describe and model these applications during the session.

9:00AM V13.00006 Explain the latent heat and specific heat of water, ammonia, and methanol with degrees of freedom. LIANYI MA, Blinn College — There are 15 known crystalline solid phases of water and all of them are called ice. But here the ice in our context is the one when water is cooled down to 0 °C at 1 atmosphere. It is well known that at 0 °C and 1 atmosphere, the density of water is 0.9998 g/cm3 and the density of ice is 0.9162 g/cm3. Question: For 0 °C water and ice, which has a higher internal energy? Because they have same temperature, their molecules should have same kinetic energies. Therefore their potential energies among molecules need to be compared. Because ice’s density is lower so it should have larger potential energy, which indicates an incredible conclusion that ice has higher internal energy. How do we explain this paradox? The internal energies of 0 °C water and ice are considered from the perspective of degree of freedom and latent heat of fusion of water is calculated, which is in good agreement with the published value. With the same consideration, the latent heats of fusion of ammonia and methanol are calculated and the results are in reasonable agreement with the published values. This simple strategy can give specific heats of water, liquid ammonia, and methanol, which are in good agreement with known data.
9:12AM V13.00007 Introducing Raman Spectroscopy of Crystalline Solids in the Undergraduate Curriculum, BAHRAM ROUGHANI, Kettering University, DAVID WARNER, UMA RAMABADRAN, Kettering University — We describe an experiment designed as an upper level physics laboratory that introduces students to Raman Scattering of electronic materials and research methodology. This experiment is an effective approach in demonstrating the relationship between the Raman intensity of the scattered light from crystals and symmetry dependent Raman selection rules. In our measurements we alter the angle between the crystal axis and the polarization of the incident laser beam by sample rotation. The three dimensional plot of the intensity profile versus the theoretical model is used to distinguish between various crystal plans of the same electronic material. This experiment combines knowledge regarding properties of materials with optical characterization. It is suitable as an upper level physics laboratory or for introducing new graduate student to use Raman spectroscopy as a research tool.

9:24AM V13.00008 Civic Engagement through Differential Equations?SHAFIQUUR RAHMAN, Allegheny College, Meadville, PA 16335 — A civic society such as ours, optimal allocations of limited resources frequently require a clear understanding of the sciences. However, policy makers often lack background in this area, and physics majors almost never get exposed to ideas that lie at the intersection of science and society, certainly not in a quantitative way. As a result, the latter show little interest in such issues. To address this problem, we have developed a short course titled Civic Engagement for Physicists. A substantial part of the course is quantitative. For example, when covering issues connected to energy, a topic of major current interest, we use a differential equation from population dynamics to study predictions about when the peak in world oil production might occur, and what the true amount of world oil reserve might be. On the other hand, topics such as Characteristics of Science and National Science Policy are covered in a qualitative way. In this talk, I’ll present details of both the quantitative and the qualitative areas covered by the course, as well as reaction of students.

1Supported by a Civic Engagement Grant from The Center for Political Participation at Allegheny College.

9:36AM V13.00009 Challenges and opportunities of undergraduate research, DANIELA M. TOPASNA, GREGORY A. TOPASNA, Virginia Military Institute — Undergraduate research at small schools is becoming the norm rather than the exception that it was years ago. Faculty are now faced with the challenges of incorporating students with varying degrees of academic preparedness and motivation in their research. This coupled with the students’ own constraints within the academic schedule can make undergraduate research a challenge for both students and faculty. Like many small undergraduate schools, VMI’s faculty and students are faced with these obstacles when engaging in undergraduate research. However, such difficulties can lead to creative solutions that lead to multiple benefits for students and faculty mentors. We present our unique perspective and experiences for this challenging yet rewarding experience as related to thin film research performed at VMI.

9:48AM V13.00010 Reacting to Galileo: Introducing a New Approach for Gen Ed Science, MICHAEL PETTERSEN, Washington and Jefferson College — Either Galileo was right, or he was wrong; either way, why was there ever any debate about it? And why should we care today about the opposing ideas, which proven wrong so long ago? In the “Reacting to the Past” series of curricular materials, students engage with key turning points in human intellectual history by taking sides and recreating the original debate. In this way, students personally identify with points of view that they would otherwise find wrong, boring, and incomprehensible — and they learn how we test ideas by challenging them, and defend them by marshalling evidence, which is the core of critical thinking. Students almost universally report that the “Reacting” experience is tremendously engaging. I shall describe an application of the “Reacting” format to the case of Galileo. The scientific issues involved are comprehensible to non-science majors, the cultural context of Renaissance Italy is rich and wonderful, and Galileo’s personal history is tremendously moving. The materials include labs designed to be taught by non-scientists teaching cross-disciplinary liberal arts courses. Other “Reacting” science materials have been published or are under development.

10:00AM V13.00011 Flint and the British Tradition of Relativity Theory, JAMES BEICHLER, Semi-retired — Most scientists and scholars are familiar with Sir Arthur Eddington’s role in verifying General Relativity in 1919. A few less are aware of his work introducing the theory to the English scientific community. Still less know of Eddington’s extensions of relativity theory, especially his attempts to develop a unified field theory. But very few scholars, historians or even physicists are aware of the important role played by other English scientists in the acceptance and development of relativity. In fact, H.T. Flint and his colleagues published more than thirty-five articles in peer reviewed journals in Britain over a period of four decades in an attempt to extend relativity to include electromagnetism and the quantum. Yet his work and that of his close associates is almost completely unknown today, in spite of the fact that he published a book describing his complete unified field theory in the 1960s, well before most quantum theorists even began thinking along the lines of unification. In a world filled with speculations about gravitons, superstrings, quantum loops and other unification models, Flint did it first, but his work has all but disappeared from the scientific consciousness. From Eddington to Flint, the English school of relativists has produced ardent supporters of relativity and numerous advances beyond the standard interpretations of general relativity.

10:12AM V13.00012 Ukrainian Physical-Technical Institute (UFTI) in the 1930’s, D.H. MCNEILL, Consultant, 3955 Bigelow Blvd., Pittsburgh, PA 15213, YU. N. RANYUK, O.S. SHEVCHENKO, Kyhrik Inst. of Physics and Technology, Ukraine — UFTI (Ukrainian Physical-Technical Institute; now Kharkiv Institute of Physics and Technology, KhFTI), founded in 1928, was among the first national laboratories. In the 1930’s, L. Shubnikov, B. Podolsky, G. Placzek, L. Tisza, F. Houtermans, A. Weissberg, V. Weisskopf, and others worked there on important and interesting research in many areas (low-temperature, electronics, nuclear physics, theory). 2008 was the centenary of Lev Landau, who established his school of theoretical physics and began his Course of Theoretical Physics in Kharkiv. It is now ~70 years since the Great purge at UFTI (and, simultaneously, throughout the USSR). UFTI’s history, a stark reminder of politics in science, is less known than that of institutions in Moscow and St. Petersburg. “Delo” UFTI 1935-1938 [The UFTI Affair, Yu. V. Pavlenko, Yu. N. Ranyuk, and Yu. A. Khramov, Kyiv, 1998] is a study, using documents available after 1990, of the lab’s early years and its near destruction in the Stalinist purges. Many scientists at UFTI were killed or imprisoned. Documents from this time will be shown. A timeline of the 1930’s at UFTI will be presented.

10:24AM V13.00013 Experience in teaching intensive course of thermal physics for undergraduate physics students, FARKHAD ALIEV, Universidad Autonoma de Madrid — This talk of non-technical nature describes experience of the author in teaching the intensive course of thermal physics for the undergraduate physics students at the Universidad Autonoma de Madrid, Spain. After brief introduction to the program, description of the WEB support of the course, I shall describe practical classes ( home-works, visits to the Laboratories, experimental demonstrations, typical problems and typical topics for presentations on the advanced thermodynamics, etc.). I shall further discuss different possible actions to wake up an interest of the students to the thermal physics and ways to simulate their active participation in the class discussions. I also describe different schemes employed in the last few years to evaluate effectively and the students work and knowledge. Finally, I will analyze the efficiency of our methodic in improving teaching of thermal physics at University level.

1Supported by Universidad Autonoma Madrid and Spanish MEC (MAT2006-07196)

Thursday, March 19, 2009 8:00AM - 10:36AM
Session V14 DFD GSNP: Disordered Systems, Glassy Dynamics, and Jamming II
8:00AM V14.00001 Specific Heat Anomalies in Glassy Fluids Due to Cluster Micro-Melting
GEORGE HENTSCHEL, Emory University, VALERY ILYIN, ITAMAR PROCACCIA, NURITH SCHUPPER, Weizmann Institute of Science — We will discuss the specific heat anomalies observed in new simulations of equimolar mixtures of particles interacting via soft core repulsive potentials under external pressure that are known to show glassy dynamics at low temperatures. The simulations show both long-lived states of microcrystalline clusters that do not nucleate a crystalline ground state and also the appearance of two specific heat peaks which were not observable in earlier simulations. We argue that the appearance of two peaks is due to the micro-melting of two types of clusters and discuss the form of the resulting specific heat anomalies. Our arguments suggest that the glass transition will typically show non-universal features.

8:12AM V14.00002 The building blocks of Dynamical Heterogeneities in dense granular media
RAPHAEL CANDELIER, OLIVIER DAUCHOT, GIULIO BIROLI, CEA — Unveiling the connection between the short term relaxation and the long term dynamical heterogeneities as observed near the glass transition in super-cold liquids and the jamming transition in granular materials remains a major challenge in the physics of glassy systems. On one hand, KMC models relate dynamical heterogeneities to a non trivial structure in the trajectory space, inherited from the local dynamical rules. On the other hand, recent studies of hard spheres close to isostaticity suggest that the collective aspect of the relaxation would stem from the extended character of the softest degrees of freedom, along which the system yields from one meta-bassin to another. There is still no direct experimental evidence in favour of one or the other mechanism in super-cold liquids nor in dense granular media. Here we will show that for a dense granular layer under cyclic shear dynamical heterogeneities result from a two timescales process. Short time but already collective events consist in clustered cage jumps, which concentrate most of the non affine displacements. Such clusters aggregate both temporally and spatially within an avalanche process, which ultimately builds the large scales dynamical heterogeneities. The typical timescale of the dynamical heterogeneities appears as the crossover between the short time separating successive event within the avalanches and the long time separating the successive jumps of any given particle.

8:24AM V14.00003 Role of Shape Anisotropy on the Glassy Dynamics of Colloidal Suspensions
MUKTA TRIPATHY, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — Center-of-mass ideal mode coupling theory (MCT), the nonlinear Langevin active particle hopping theory, and the Reference Interaction Site Model have been employed to investigate the structure and slow dynamics of suspensions composed of hard and rigid nonspherical objects. Objects of dimensionality one (rods, rings), two (discs), and three (polyhedra) have been studied. For non-compact particles the volume fraction of ideal kinetic arrest, corresponding to a crossover to activated dynamics, decreases with particle dimensionality and/or aspect ratio. On the other hand, the ideal vitrification volume fraction of compact 3-dimensional objects is a complex and subtle function of particle shape. Calculations of the entropic barrier for activated transport, mean relaxation time, transient localization length, diffusion constant, elastic modulus, and effective fragility have been performed. Deep in the ideal glassy region the barrier height and mean hopping time are controlled by the shape-dependent mean square confining force exerted on a particle by its surroundings. A nearly universal collapse of many dynamical properties is achieved based on a dimensionless difference variable that quantifies the magnitude of the mean square force compared to its critical value at the ideal MCT transition.

8:36AM V14.00004 Coupled Translational and Rotational Glassy Dynamics in Hard Dicollloid Suspensions
RUI ZHANG, KENNETH SCHWEIZER — Naive mode coupling theory (NMCT) and the nonlinear Langevin equation (NLE) theory of activated glassy dynamics have been generalized to treat the coupled center-of-mass translation and rotational motions of hard linear objects of variable aspect ratio. Two types of ideal nonequilibrium transitions are predicted corresponding to localization of only translation (plastic glass for small aspect ratios) or simultaneous arrest of translation and rotation (double glass). The NMCT kinetic arrest transition signals a crossover to activated dynamics controlled by entropic barriers. Specifically, a two-dimensional dynamical free energy surface (function of translational displacement and rotational angle) is constructed which quantifies effective rates of all process corresponding to the trajectory of lowest entropic barrier is associated with a system-specific translation-rotation cooperative motion. Mean alpha relaxation times as a function of dicollid aspect ratio and volume fraction are computed using multidimensional Kramers theory.

8:48AM V14.00005 Constitutive relations in dense granular flows
JOHN DROZD, COLIN DENNISTON, University of Western Ontario — We use simulations to investigate constitutive relations in dry granular flow. Our system is comprised of mono- and poly-disperse sets of spherical grains falling down a vertical chute under the influence of gravity. We observe three phases or states of granular matter: a free-fall dilute granular gas region at the top of the chute, a granular fluid in the middle and then a glassy region at the bottom. We test various proposed constitutive relations to provide a basis for analytically solving for the stresses in granular flows. Finally, we examine the energy conservation and heat flow in our systems and show that the heat conductivity constitutes distinct power-law dependencies on the granular temperature in the glassy and fluid regions of our system.

9:00AM V14.00006 Polytetrahedral Frustration of Crystallization: A Study of 4d Hard Spheres
PATRICK CHARBONNEAU, Duke University, JACOBUS A. VAN MEEL, FOM Institute for Atomic and Molecular Physics, DAAN FRENKEL, Cambridge University — Geometrical frustration is thought to be the supercooling of a liquid. In 3d hard spheres the preferred local cluster is isohedral and the densest packing is tetrahedral, but no periodic lattice is consistent with either symmetry in Euclidian space, so a crystal phase with a different symmetry nucleates upon compression. For 2d disks in contrast triangular or hexagonal order is both locally and globally preferred and crystallization of a metastable fluid is quasi-instantaneous. Yet the precise origin of geometrical frustration remains unclear, because in 2d and 3d polytetrahedral structures are often equated conceptually to the optimal local cluster. Here, we conduct a computational study of the 4d analogue, where the optimal local cluster and global order are commensurate, but the polytetrahedral order is not. We observe no sign of facile crystal formation, which support the polytetrahedral frustration scenario. We also find the fluid to be structurally very different from the crystal. The resulting high interfacial free energy sheds new light on 3d geometrical frustration and its role in glass formation.

9:12AM V14.00007 Noise as a Probe of Ising Spin Glass Transitions
ZHI CHEN, CLARE YU, University of California, Irvine — Noise is ubiquitous and is often viewed as a nuisance. However, we propose that noise can be used as a probe of the fluctuations of microscopic entities, especially in the vicinity of a phase transition. In recent work we have used simulations to show that the noise increases in the vicinity of phase transitions of ordered systems. We have recently turned our attention to noise near the phase transitions of disordered systems. In particular, we are studying the noise near Ising spin glass transitions using Monte Carlo simulations. We monitor the system as a function of temperature. At each temperature, we perform slow shear of colloidal glasses using a confocal microscope and shear-cell set up. The particles are tracked in time and space to construct the local strain field, which is observed to be non-uniform with high strain and low strain zones interspersed in space. Our measurements at a volume fraction ~ 58% show the existence of homogeneous sheared regime, at a shear rate ~5x10^{-15} s^{-1} and shear localization at higher shear rates (~10^{-4} s^{-1}). The set-up offers a unique opportunity to elucidate the evolution of shear-bands using the concept of shear transformations. In particular, the aim is to understand the role of correlation between the shear transformations in the growth of shear bands. We present an overview over the homogeneous versus inhomogeneous shear regime in terms of a deformation map for these systems.

Work supported by DOE grant DE-FG02-04ER46107.

9:24AM V14.00008 Shear banding in colloidal glasses
VIJAYAKUMAR CHIKKADI, University of Amsterdam, THE NETHERLANDS, ANDREW SCHOFIELD, University of Edinburgh, U.K., PETER SCHALL, University of Amsterdam, The Netherlands — We perform slow shear of colloidal glasses using a confocal microscope and shear-cell set up. The particles are tracked in time and space to construct the local strain field, which is observed to be non-uniform with high strain and low strain zones interspersed in space. Our measurements at a volume fraction ~ 58% show the existence of homogeneous sheared regime, at a shear rate ~5x10^{-15} s^{-1} and shear localization at higher shear rates (~10^{-4} s^{-1}). The set-up offers a unique opportunity to elucidate the evolution of shear-bands using the concept of shear transformations. In particular, the aim is to understand the role of correlation between the shear transformations in the growth of shear bands. We present an overview over the homogeneous versus inhomogeneous shear regime in terms of a deformation map for these systems.
9:36AM V14.00009 Correlations between Dynamical Heterogeneity and Viscoelasticity of Confined Colloidal Suspensions under Oscillatory Shear, PRASAD SARANGAPANI, YINGXI ELaine ZHU, University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN 46556 — In this talk, we present a recent rheological study of confined amorphous colloidal thin films under oscillatory shear using a home-designed micron-gap rheometer interfaced with a confocal microscope. We visualize the response of "hard-sphere" poly-(methyl methacrylate) (PMMA) particles of 1.2 µm in diameter to applied shear deformation and simultaneously measure the viscos and elastic moduli of PMMA colloidal thin films of bulk volume fraction, φ = 0.430-0.57, confined at gaps ranging from 50 µm to 1.2 mm. For confined PMMA colloids under shear at gaps where an applied deformation is sufficiently large to induce non-linear responses, we find commonality in particle dynamics where strongly non-affine motion causes particles to move as cooperatively rearranging groups. However, on average the length scale of these groups is larger than the typical length scales of dynamical heterogeneities for the un-sheared thin films and typically approaches the order of confining dimension. We quantify the nature of shear induced flow cooperativity and its relation to a shear thickening transition observed in the limit of large strain amplitudes.

9:48AM V14.00010 Aggregation of athermal particles induced by capillarity, MICHAEL BERHANU, ARSHAD KUDROLLI, Department of Physics, Clark University, Worcester, MA 01610. — Aggregation of cohesive particles floating in a medium is a very broad physical phenomena occurring in colloidal systems, soot particles, and intergalactic dust under gravitation. We investigate the geometrically constrained dynamics of aggregation with new experiments using floating spheres at the air-water interface. A short range attractive force can be induced by careful choice of buoyancy and capillarity to create self-assembled particle structures which can be tracked by imaging. First, the particles are placed randomly at the interface, and then aggregation is induced by smoothly decreasing the area of the interface which causes the particles to come within the attractive force range caused by capillarity. We measure the area fraction at which the connectivity and rigidity percolation transitions are observed and further characterize the aggregates with two-point correlation functions. We then compare and contrast our results with gelation and jamming transitions reported with colloids and granular matter. Finally, we study the reverse phenomena, where we probe the response of the aggregate to an increase in interface area.

10:00AM V14.00011 Correlation range in a supercooled liquid via Green-Kubo expression for viscosity, local atomic stresses, and MD simulations, VALENTIN A. LEVASHOV, TAKESHI EGAMI, JAMES R. MORRIS, University of Tennessee and Oak Ridge National Laboratory — We present a new approach to the issue of correlation range in supercooled liquids based on Green-Kubo expression for viscosity. The integrand of this expression is the average stress-stress autocorrelation function. This correlation function could be rewritten in terms of correlations among local atomic stresses at different times and distances. The features of the autocorrelation function decay with time depend on temperature and correlation range. Through this approach we can study the development of spatial correlation with time, thus directly addressing the question of dynamic heterogeneity. We performed MD simulations on a single component system of particles interacting through short range pair potential. Our results indicate that even above the crossover temperature correlations extend well beyond the nearest neighbors. Surprisingly we found that the system size effects exist even on relatively large systems. We also address the role of diffusion in decay of stress-stress correlation function.

10:12AM V14.00012 Dynamics in Complex Fluids Formed by Conjugated Polymers, NAresh OSTI, Department of Chemistry, Clemson University, Clemson, SC 29634, MADHUSUDAN TYAGI, NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, DILRU RATNAWEERA, Department of Chemistry, Clemson University, Clemson, SC 29634, UWE BUNZ, Department of Chemistry and Biochemistry Georgia Institute of Technology, Atlanta, GA 30332, DVORA PERAHIA, Department of Chemistry, Clemson University, Clemson, SC 29634 — Alkyl di-substituted para-polyphenyleneethylene (PPE) associates into several complex fluids in dilute solutions of toluene. At high concentrations these molecules are strongly flattened, associating in the direction perpendicular to the long molecular axis. At the temperature of the glass transition the molecules associate and eventually jam to a fragile gel. These phases are optically active where the dynamic processes affect their optical characteristics. Inelastic Neutron Back Scattering conjunction with Neutron Spin Echo was used to characterize the dynamics on multiple length scales at different temperatures. The current talk will introduce the neutron backscattering results that follow internal dynamics within the PPE molecules as they are confined into aggregates and jams to form a fragile phase. The data will be discussed in terms of Kohlrausch-Williams-Watt model that provides characteristics time constants for the different dynamic processes.

10:24AM V14.00013 Spontaneous transition in TiNiFe strain glass system, JIAn ZHANG, XIAOBING REN, YU WANG, KAZUHIRO OTSUKA, JUN SUN, Multi-disciplinary Materials Research Center, Xi an Jiaotong University,710049, P.R. China; Ferroic physics group, NIMS, Tsukuba, Japan — Glass has been considered as one major challenge for the statistic mechanics, for the presumption of ergodicity is no longer valid. Hence, glass transition was normally viewed as solely kinetic driven process, including ferroic cluster glasses. Whereas, the ferroic cluster glasses appear once the thermodynamics driven ferroic phases are suppressed by the point defects. It seems quite intriguing why the power of thermodynamics is immediately rewritten in terms of correlations among local atomic stresses at different times and distances. Through this approach we can study the development of spatial correlation with time, thus directly addressing the question of dynamic heterogeneity. We performed MD simulations on a single component system of particles interacting through short range pair potential. Our results indicate that even above the crossover temperature correlations extend well beyond the nearest neighbors. Surprisingly we found that the system size effects exist even on relatively large systems. We also address the role of diffusion in decay of stress-stress correlation function.

Thursday, March 19, 2009 8:00AM - 10:48AM — Session V15 DFD: Liquid Crystals I 316

8:00AM V15.00001 Interaction and Response of a Smectic-A liquid crystal to a 2 nm Nanometer Particle: Phase transition due to the Functionalization Compound, LUZ J MARTINEZ-MIRANDA, University of Maryland, LYNN K KURIHARA, Naval Research Laboratories — We have studied the in-plane (parallel to the magnetic field) alignment of 8CB mixed with FeCo nanoparticles covered with different functionalization compounds. The functionalization compounds are Polyethylene glycol (PEG (3000)), hydroxyl succinimide (NHS), aminopropyl tri-ethoxy silane (APTS) and mercapto hexa-decanoic acid (MHD). We have studied them using X-ray scattering. We have found that the inverse integrated intensity of the X-ray scans in the plane of the magnetic field is a good measure of how much energy the system (liquid crystal, nanoparticles, functionalization compound) will need to reorient the liquid crystal in the magnetic field. In addition, we have observed that the orientation the liquid crystal adopts with respect to the nanoparticles can result in a phase transition that takes the liquid crystal to a more disordered and symmetric phase that favors the rotation, as happens in the smectic-nematic transition, observed in the sample with APTS. We relate the disordering to the changes observed in the transition for the liquid crystal and this termination to recent heat capacity measurements by Cordoyiannis et al. [1].

8:12AM V15.00002 Theory of Ferroelectric Nanoparticles in Nematic Liquid Crystals, LENAPATINA, JONATHAN SELINGER, Liquid Crystal Institute, Kent State University. Many recent experiments have reported that ferroelectric nanoparticles have drastic effects on nematic liquid crystals. Low concentrations of such particles increase the nematic-isotropic transition temperature by over 10 °C, and greatly increase the sensitivity of the nematic phase to applied electric fields. To understand these effects, we develop a theory for the statistical mechanics of ferroelectric nanoparticles in liquid crystals. In this theory, the key issue is the distribution of orientations for the electrostatic dipole moments of the nanoparticles. This distribution is characterized by an orientational order parameter, which interacts with the orientational order of the liquid crystals and stabilizes the nematic phase. We estimate the coupling strength and calculate the resulting enhancement in the transition temperature, in good agreement with experiments. We also predict the response to applied electric fields, showing that the Kerr effect is enhanced above the isotropic-nematic transition. These predictions apply even when the electrostatic interactions are partially screened by moderate concentrations of ions.

3Work supported by NSF Grant DMR-0605889.

8:24AM V15.00003 Unconventional dimerization in mesogenic semi-phasmidic type carboxylic acid*, SHIN-WOONG KANG, SEUNG-YEON JEONG, DENA MAE AGRA-KOOLJAN, SATYENDRA KUMAR, Department of Physics, Kent State University, VEENA PRASAD, SANJAY VARSHNEY, Centre for Liquid Crystal Research, Bangalore, INDIA. Nematic and columnar mesophases formed by a semi-phasmidic type carboxylic acid are investigated by DSC, X-ray scattering, FTIR spectroscopy, and polarizing optical microscopy. FTIR spectroscopy and X-ray diffraction reveal that two semi-phasmidic type carboxylic acid molecules form a mesogenic dimer through inter-molecular hydrogen bonding. X-ray diffraction results obtained under in-situ magnetic field reveal unique characteristics that set them apart from conventional linear dimers formed via hydrogen bonding. These dimers possess negative dielectric and diamagnetic anisotropies. Values of the length scales corresponding to the diffraction peaks and their orientation relative to the magnetic field strongly suggest the formation of a “bent-core-like” mesogenic dimers rather than conventional coplanar linear dimers.

4Supported by grant NSF/DMR-060991.


8:48AM V15.00005 The shape and conformation of the mesogenic group in tetrapodic liquid crystals, HYUNGYOUNG YOON, SHINWOONG KANG, Department of Physics, Kent State University, GEORGE H. MEHL, Department of Chemistry, University of Hull, UK, SATYENDRA KUMAR, Department of Physics, Kent State University. The nematic mesophases formed by tetrapodic mesogens based on Si- or Ge-core have been investigated by various methods [1]; deuterium NMR, polarized IR spectroscopy, and light scattering. In these studies, biaxiality of the nematic phase has been a central issue. The average statistical shape of such a complex molecule adopts and how the four mesogens attached to Si/Ge atom are oriented in the nematic and lower temperature phases are naturally important questions. However, these have not been sufficiently discussed. We performed synchrotron x-ray diffraction experiments on magnetic aligned Ge-tetrapodes, augmented by conoscopy, capacitance, and electro-optical experiments. The results of these studies and the inferences drawn for the mesogenic group formation will be presented. [1] K. Neupane, S.W. Kang, S. Sharma, D. Carney, T. Meyer, G. H. Mehl, D.W. Allender, S. Kumar, and S. Sprunt, Phys. Rev. Let. 97, 207802 (2006), and references there in.

Work supported by grant NSF/DMR-080991.

9:00AM V15.00006 Quantum dot dispersion in nematic liquid crystal, J. KIRCHHOFF, Florida State University, ROBERT INMAN, D.S. CHANDHOK, S. GHOSH, L.S. HIRST, University of California Merced. Optical and electrical properties of quantum dots can be significantly altered by aligning the dots in a linear chain. Dispersing quantum dots in liquid crystals can lead to the formation of linear chains due to the partial ordering of the liquid crystal molecules. Typically, this results in a red shift in the emission spectrum of the dots as the induced order leads to enhanced dipolar interactions, resulting in electronically coupled states. Dispersions of quantum dots are studied as a function of the concentration, size, and shape of the dots in a nematic rod-like liquid crystal material. The quantum dots are seen to aggregate if the concentration of the dots is too high, leading to enhanced dipolar interactions, resulting in electronically coupled states. Dispersions of quantum dots are studied as a function of the concentration, size, and shape of the dots in a nematic rod-like liquid crystal material. The quantum dots are seen to aggregate if the concentration of the dots is too high, leading to little correlation between the quantum dot dispersion and liquid crystal texture. In decreasing the quantum dot concentration the aggregates lessen in size and are more uniformly distributed within the liquid crystal. Spherical, rod-like, and disc-like quantum dots with emission peaks ranging from 490 nm to 640 nm were studied using polarized optical microscopy and scanning microscopy photoluminescence measurements.

9:12AM V15.00007 Dielectric and Optical Properties of Nematic ODBP-Ph-C7*, BOHDAN SENYUK, HUGH WONDERLY, SERGIY SHIYANOVSKII, OLEG LAVRENTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, VICTOR P. PENGAMENSHCHIK, Display and Semiconductor Physics, Korea University, Kangwon 339-700, South Korea; Institute of Physics, Prospect Nauky 46, Kyiv 03039, Ukraine. Thermotropic biaxial nematic liquid crystals are promising for application in fast switching electro-optical devices. In the present work, we study the optical and dielectric properties of the nematic phase of thermotropic LC material, 4,13,6(3,4-x-dioxadiol2,5-diyl) diphenylbenzoate (ODBP-Ph-C7) with boomerang-like molecules, reported to exhibit the biaxial nematic phase [2]. We study ODBP-Ph C7 in well-aligned "monocristalline" states. The experiments show that the uniaxial and dielectric properties of the material, such as high dielectric dispersion and dielectric relaxation times increase with temperature. We also analyze defect structures formed by ODBP-Ph-C7 in different geometries of confinement and boundary conditions. [1] G. R. Luckhurst, Thin Solid Films 393, 40 (2001); 2 B. R. Acharya, A. Primak, T. J. Chengmans, E.T. Samulski and S. Kumar, Pramana J. Phys. 61, 231 (2003).

Supported by NSF Grant DMR-0504516 and DOE grant DE-FG02-06ER46314.

9:36AM V15.00009 Theory and simulation of two-dimensional nematic and tetragonic phases1 . JUN GENG, JONATHAN V. SELINGER, Liquid Crystal Institute, Kent State University — Recent experiments and simulations have shown that two-dimensional systems can form tetragonic phases with four-fold rotational symmetry, even if they are composed of particles with only two-fold symmetry. To understand this effect, we propose a model for the statistical mechanics of particles with almost four-fold symmetry, which is weakly broken down to two-fold. We introduce a coefficient \( \kappa \) to characterize the symmetry breaking, and find that the tetragonic phase can still exist even up to a substantial value of \( \kappa \). Through a Landau expansion of the free energy, we calculate the mean-field phase diagram, which is similar to the result of a previous hard-particle exclusion-volume model. To verify our mean-field calculation, we develop a Monte Carlo simulation of spins on a triangular lattice. The results of the simulation agree very well with the Landau theory.

1This work was supported by NSF Grant DMR-0605889.

9:48AM V15.00010 Quadrupolar particles in a nematic liquid crystal: Effects of particle size and shape . FRANCISCO HUNG, Cain Department of Chemical Engineering, Louisiana State University — We investigate the effects of particle size and shape on the quadrupolar (Saturn ring-like) defect structures formed by a nematic liquid crystal (NLC) around nm- and micron-sized particles with spherical, spherocylindrical and cubic shapes. Our calculations, based on a Landau-de Gennes expansion in terms of the tensor order parameter \( \mathbf{Q} \), indicate that for pairs of nanoparticles in close proximity, the most stable defect structure is the "entangled hyperbolic" [1]. For pairs of micron-sized particles the NLC forms entangled "figure of eight" defects [1] around pairs of spheres and spherocylinders. In contrast, we only observed unentangled defect structures around pairs of micron-sized cubic particles. For pairs of spherical and spherocylindrical particles, the transition between "entangled hyperbolic" and "figure of eight" structures occurs when the particle diameter is between 100 nm and 1 micron. Our calculations suggest that the NLC-mediated interactions between the nanoparticles are fairly strong (up to 5700 kT). These interactions can bind the particles together at specific locations, and thus could be used to assemble the particles into ordered structures with different morphologies. [1] M. Ravnik et al., Phys. Rev. Lett. 99, 247801 (2007)

10:00AM V15.00011 A Model Liquid Crystalline System Based on Rodlike Viruses with Tunable Chirality , DANIEL BELLER, EDWARD BARRY, ZVONIMIR DOGIC, Brandeis University — Filamentous bacteriophages such as the fd virus have long been used as ideal model systems to investigate the phase behavior of suspensions of rodlike particles. We study the structure and phase behavior of a mutant, fd Y21M, and compare them to the properties of conventional fd wild-type (wt). These two viruses exhibit dramatically different phase behavior despite differing only by a single amino acid of the major coat protein pVII. We find that this is attributable to significant differences in the flexibility of the viruses. Using the more rigid fd Y21M, we are able for the first time to quantitatively test the Onsager description of the isotropic-nematic phase transition of rigid rods. Even more surprising are the differences in the behavior of the cholesteric phase of fd Y21M and fd wt. While fd wt forms a cholesteric pitch with a left-handed helix, fd Y21M forms a cholesteric pitch with the opposite handedness. In addition, the magnitude of the cholesteric pitch changes by almost fivefold. Using mixtures of the two viruses, we are able to create liquid crystal systems with tunable control over the macroscopic chiral behavior.

10:12AM V15.00012 Apparent Broken Reciprocity in Chiral Liquid Crystals1 , MICHELE MOREIRA, NITHYA VENKATARAMAN, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, LORENZO MARRUCCI, Dipartimento di Scienze Fisiche, Università di Napoli "Federico II" — Reciprocity in optics is predicated on bounded scattering media with symmetric and linear permittivity, conductivity and permeability. Due to their anisotropy and chirality, cholesteric liquid crystals (CLCs) form periodic dielectric structures. If the periodicity is comparable to the wavelength of light, these phases are self-assembled photonic band gap structures. There appear in the permittivity odd powers of the wave vector resulting from nonlocality and broken inversion symmetry. Evidence of non-reciprocity has been found in optically active crystals by Bennett [1] and in stacks of cholesteric and nematic liquid crystal cells by Takezoe [2]. We investigate experimentally and theoretically the possibility of a violation of optical reciprocity of a hetero-photonic-bandgap structure made of two CLC cells of different pitch. We have observed a significant apparent violation, but we show that the effect is due to light scattering, and in fact these cholesteric structures are reciprocal.

1This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

10:24AM V15.00013 Raman scattering study of orientation order parameters in thermotropic biaxial nematic LC , MIN SANG PARK, BUM JIN YOON, JUNG OK PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, Atlanta, GA, USA, VEENA PRASAD, Center for Liquid Crystal Research, Bangalore, India , MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, USA — There has been considerable interest in the liquid crystalline phases formed by bent-core molecules, since these molecules were considered to have a biaxial nematic phase. In an effort to understand the orientation behavior and the degree of phase biaxiality in bent-core mesogens, Raman spectroscopy has been used to measure the scattering intensities for orthogonal linear polarization. This straightforward methodology allows the values of both uniaxial, \( \langle P_{200} \rangle \) and \( \langle P_{400} \rangle \), and biaxial order parameters, \( \langle P_{220} \rangle \), \( \langle P_{202} \rangle \), and \( \langle P_{410} \rangle \) to be quantified. From experimentally derived order parameters, the most probable orientation distribution functions are constructed. The results of these measurements will be presented in the context of experimental evidence of phase biaxiality obtained by other methods including X-ray diffraction and NMR.

10:36AM V15.00014 Liquid crystalline behaviors of H-bonded dimer formed from the semi-phasicdride type carboxylic acid * , SEUNG-YEON JEONG, SHIN-WOONG KANG, SATYENDRA KUMAR, Department of Physics, Kent State University, VEENA PRASAD, SANJAY VARSHNEY, Centre for Liquid Crystal Research, Bangalore, INDIA — Liquid crystalline properties of acid-functionalized semi-phasicdride azo-compound were characterized by DSC, polarizing optical microscopy, and electro-optical measurements. The results suggested that this unconventional mesogen has a non-typical effective "bend" angle where two monomers form the hydrogen bond. To confirm this, we performed electro-optical experiments in the nematic phase with strong external electric and magnetic fields. Cells with different surface geometries and treatments we used. The results reveal a behavior that is very distinct from that expected of conventional linear mesogenic dimers formed by a hydrogen bonding. The results confirm negative values of dielectric and diamagnetic anisotropies. Our observations indicate that "bent-like" dimeric mesogens are formed through an unconventional inter-molecular association. *Work supported by grant NSF/DMR-086991.

Thursday, March 19, 2009 8:00AM - 10:24AM – Session V16 DCMP: Solid Helium: Experiment 317
8:00AM V16.00001 Bose-Einstein condensation in solid helium, RICHARD AZUAH, NIST Center for Neutron Research, Gaithersburg, SOULEYMANE DIALLO, Ames Laboratory, Ohio, OLEG KIRICHEK, ISIS Spallation Neutron Source, Didcot, UK, HENRY GLYDE, University of Delaware — We report new measurements of the Bose-Einstein condensate fraction in solid helium. The goal is to reveal whether there is BEC associated with the superfluid fractions that have been observed in solid helium [1,2]. The condensate fraction, n_0, is obtained from neutron scattering measurements of the momentum distribution, n(k), of the atoms in the solid. We use commercial grade helium (^{4}He concentration of 0.3 %) where the T_c for superflow is T_c = 200 mK and have measured the n(k) at 3 temperatures, 500 mK, 150 mK and 65 mK. We use a sample cell that has a large surface to volume ratio (S/V) ≈ 40 cm^{-1} where large superfluid fractions have recently been reported[2]. We use a large sample volume (100 cm^3) and high instrument resolution to improve precision beyond that of previous measurements [3]. No clear sign of BEC has been observed but the data is being analyzed so that specific values of n_0 can be reported. [1] E. Kim and M.H.W. Chan, Science, 305:1941 (2004); Nature, 427:225, 2004. [2] A. S. C. Rittner, and J. D. Reppy, Phys. Rev. Lett., 98:175302, 2007. [3] Díallo et al. Phys. Rev Lett. 98, 205301 (2007).

8:12AM V16.00002 Pressure-driven mass flow in solid 4He, ANN SOPHIE C. RITTNER, Department of Physics and Astronomy and Rice Quantum Institute, Rice University, Houston, TX 77251, USA, WONSUK CHOI, Physics Department, KAIST, Daejeon, South Korea, JOHN D. REPPY, Laboratory of Atomic and Solid State Physics and the Cornell Center for Materials Research, Cornell University, Ithaca, NY 14853, USA — We report on two experiments that explore pressure-driven flow in solid 4He. In the first experiment, two pancake-shaped chambers are connected by a narrow slit. The pressure in one chamber is varied periodically at 2 mHz and we look for a superfluid pressure response in the second chamber. When the cell is filled with liquid, we observe a large pressure signal in the second chamber as expected for superfluid flow. In solid helium, no pressure response is detected outside the noise level. In a second experiment, we generate an oscillating pressure in a torsional oscillator by blocking an annulus. We expect the pressure difference to drive the supersolid component through a radial channel orthogonal to the rotational motion of the oscillator.

1Supported by NSF Grants DMR-0203244 and DMR-0520404

8:24AM V16.00003 Observation of Mass Flux through solid 4He, ROBERT HALLOCK, MICHAEL RAY, Univ. of Mass. Amherst — We have developed a novel apparatus and technique that allows us to maintain an interface between superfluid helium and hcp solid 4He at pressures greater than ≈ 25 bar, the low temperature solid-liquid coexistence pressure. We use this apparatus to inject helium into one side of the solid, creating a chemical potential difference across the solid, and we then look for a response in the pressure on the other side. We observe a flux of atoms through the solid[1] which tends to decrease with increasing solid pressure. There is also a complicated temperature dependence, which suggests hysteretic behavior. We will describe the experimental apparatus, and some of our results.


1Supported by the NSF

8:36AM V16.00004 Growth of hcp Solid 4He from the Superfluid, MICHAEL RAY, ROBERT HALLOCK, Univ. of Mass. Amherst — Using the same experimental apparatus that we developed to search for mass flux in hcp solid 4He at pressures greater than 25 bar[1], we study the growth of solid helium from the superfluid at constant temperature. As the pressure of the solid is driven above the melting curve, with helium continuously being added to the sample cell, we observe apparently random events during which the pressure of the solid drops. These pressure drops are accompanied by a sharp transient rise in the temperature of the cell. We will present the data, along with some discussion of what might cause these transients.


1Supported by the NSF

8:48AM V16.00005 Velocity dependence of supersolid He-4 in a torsion oscillator, ETHAN PRATT, BENJAMIN HUNT, VIKRAM GADAGKAR, Cornell University, MINORU YAMASHITA, Kyoto University, J.C. SEAMUS DAVIS, Cornell University, Brookhaven National Laboratory, University of St. Andrews — We have developed a free-inertial-decay mapping technique which allows us to acquire the complete velocity-temperature phase diagram of supersolid He-4. A striking new feature of the resulting supersolid response map is the appearance of an enhanced dissipation superpeak. We discuss these results in context of various microscopic mechanisms for the velocity-induced suppression of the supersolid response, including a superfluid critical velocity, defect network critical shear, and a glassy dynamical susceptibility.

9:00AM V16.00006 Torsional oscillator measurements on solid helium in a partially blocked annular channel, DUK YOUNG KIM, SANG-IL KWON, HYOUNGSOON CHOI, EUNSEONG KIM, KAIST, CSQR AND DEPARTMENT OF PHYSICS TEAM — We employed a torsional oscillator technique to investigate the non-classical response of solid helium. We grow solid helium samples within an annular channel that is divided by two Vycor blocks. The melting pressure of helium in narrow pores of Vycor glass is elevated up to about 37 bar due to partial blocking the pressure. This work is supported by Creative Research Initiative of MOST/KOSEF.

9:12AM V16.00007 Simultaneous Oscillation of Annular Solid 4He Samples at Two Mode Frequencies in Compound Torsion Pendulum, MICHAEL C. KEIDERLING, HARRY KOJIMA, Rutgers University — We have extended our studies on the non-classical behavior of solid 4He contained in compound torsional oscillator (TO) cell below 1 K. Our unique TO design allows observations on the identical sample at two distinct frequencies (f_1=493 and f_2=1165 Hz). The sample was grown by blocked capillary method in an annular cell(id = 8.0 mm, od = 10.0 mm, height = 9.0 mm). We focus here on experiments in which the two modes are excited simultaneously. While keeping the drive of f_1 mode at a very low level, the drive of f_2 mode was varied from high to low levels to produce substantial variations in the non-classical rotation inertia fraction (NCRIf). When the NCRIf seen by f_1 mode is reduced by 89, 91 and 94 % at 9.7, 23.5 and 56.5 mK, respectively, the NCRIf seen by f_2 mode (driven at low level) is reduced by 62, 68 and 80 %. The discrepancies and their temperature dependence in the observed reductions in NCRIf are not yet understood. Similar Measurements with the roles of the drive levels of the modes reversed as well as the changes in the dissipation of the torsional oscillator during the simultaneous drive will be reported.

3Supported in part by NSF grant DMR-0704120.
9:24AM V16.00008 Effects of $^3$He Impurities on the Non-Classical Rotation Inertia of Solid $^4$He as Measured by Compound Torsion Pendulum, DAVID RUFFNER, MICHAEL KEIDERLING, PATRYK GUMANN, HARRY KOJIMA, Rutgers University — An intriguing observation related to the discovery of non-classical rotational inertia (NCRI) of solid $^4$He at low temperatures is the extreme sensitivity to $^3$He concentration ($x_3$). Both the magnitude and temperature dependence of the NCRI are affected by relatively low $x_3$ introduced into solid $^4$He samples.[1] We are exploring the $^3$He impurity effect using our compound torsional pendulum which allows probing the NCRI of the identical solid $^4$He sample at two different frequencies (~493 and ~1165 Hz). The NCRI fractions were derived from the measured shifts in the oscillator frequency of the two modes as functions of temperature. The NCRI fraction derived from the higher frequency mode is greater than that derived from the lower frequency mode at all temperatures. If the NCRI fractions of both modes are normalized at their maximums, the temperatures at which they decrease to 50 % of the maximum are greater in the higher mode by ~9, 31 and 56 mK when the nominal $x_3$ added is 0.3, 3 and 10 ppm, respectively. Greater values of $x_3$ are currently being studied.[1]Kim, et al., Phys. Rev. Lett. 100 065301(2008).

1Supported in part by NSF grant DMR-0704120.

9:36AM V16.00009 Sample quality dependence of the specific heat peak in solid $^4$He, XI LIN, Z. G. CHENG, M. H. W. CHAN, Penn State U. — We reported a broad peak in specific heat of solid $^4$He at low temperatures is the extreme sensitivity to $^3$He concentration ($x_3$). Both the magnitude and temperature dependence of the NCRI are affected by relatively low $x_3$ introduced into solid $^4$He samples.[1] We are exploring the $^3$He impurity effect using our compound torsional pendulum which allows probing the NCRI of the identical solid $^4$He sample at two different frequencies (~493 and ~1165 Hz). The NCRI fractions were derived from the measured shifts in the oscillator frequency of the two modes as functions of temperature. The NCRI fraction derived from the higher frequency mode is greater than that derived from the lower frequency mode at all temperatures. If the NCRI fractions of both modes are normalized at their maximums, the temperatures at which they decrease to 50 % of the maximum are greater in the higher mode by ~9, 31 and 56 mK when the nominal $x_3$ added is 0.3, 3 and 10 ppm, respectively. Greater values of $x_3$ are currently being studied.[1]Kim, et al., Phys. Rev. Lett. 100 065301(2008).

This work is supported by NSF Grants DMR-0706339.

9:48AM V16.00010 Torsional oscillator and specific heat studies of 4He in Vycor, Z.G. CHENG, X. LIN, J.T. WEST, M.H.W. CHAN, Penn State University — Non-classical rotational inertia (NCRI) was first reported in solid helium confined in Vycor using the torsional oscillator technique [1]. Most of the work since then has focused on bulk solid helium. Recent specific heat measurements of bulk solid helium show a peak centering near the NCRI onset temperature [2], a good indication that the two may be related. We report on a series of experiments to study the NCRI fraction and specific heat of solid helium in Vycor. The torsional oscillator experiment is revisited to study the stability of the NCRI fraction. The purpose of the specific heat measurement is to probe the relation between the specific heat peak and NCRI.


The work is supported by NSF Grants No. DMR-0706339.

10:00AM V16.00011 Second sound in supersolid $^4$He, NORBERT MULDERS, Department of Physics, University of Delaware, SANGIL KWON, EUNGSEONG KIM, Center for Supersolid Quantum Matter Research and Department of Physics, KAIST, Korea — In a system that consists of two interpenetrating continuous phases that are free to move with respect to each other, one would expect to find two longitudinal sound modes. A good example is fourth sound in superfluid helium in a porous matrix, but the phenomena can also be observed with water in rocks. If one interprets the observation of a non-zero NCRI in solid helium below ~100 mK as due to the independent motion of a supersolid fraction with respect to the crystal, it follows that two longitudinal sound modes should exist, with the slow mode disappearing at the supersolid transition. We will report on our efforts to find this slow mode.

10:12AM V16.00012 Supersolidity of Solid $^4$He Confined in 25 Angstrom Nanopores, KEIYA SHIRAHAMA, HITOMI YOSHIMURA, YOSHIYUKI SHIBAYAMA, Keio University — There has been growing consensus that dislocations play an important role on the supersolid behaviors observed in torsional oscillator experiments for solid $^4$He. When solid He is confined in nanopores, dislocations may not exist, or even if they exist their motion is suppressed, and supersolidity should therefore be greatly modified. Study of solid $^4$He in confined geometries may therefore give an important clue to elucidate the mechanism of supersolidity. Earlier studies of solid $^4$He in Vycor by Kim and Chan [1] found no difference in the supersolid behaviors from bulk solid. We have performed torsional oscillator experiments for solid $^4$He in a porous Gelsil glass that has nanopores of 25 angstroms in diameter. We have observed an increase in oscillator frequency indicating supersolidity below 200 mK. This result suggests that the existence of dislocations is not a necessary condition for supersolidity. [1] E. Kim, M. H. W. Chan, Nature 427, (2004) 225.

Work supported by Grant-in-Aid for Scientific Research on Priority Area, MEXT, Japan

Thursday, March 19, 2009 8:00AM - 11:00AM – Session V17 GQI: Superconducting Transmons and Circuit QED

8:00AM V17.00001 Experimental study of transmon type qubits coupled to a fast tunable transmission line resonator, MARTIN SANDBERG, CHRIS WILSON, FREDRIK PERSSON, IO-CHUN HOI, PER DELSING, Chalmers University of Technology — We experimental study a high quality factor (Q-value) transmission line resonator terminated in a superconducting quantum interference device (SQUID). Using an on-chip fast flux bias line we show that we can tune the frequency of such a resonator by hundreds of line widths on a time scale faster the photon lifetime of the resonator. Such a resonator could then be used for dynamic coupling of superconducting quantum bits (qubits). We present preliminary data of two transmon type of qubits coupled to a fast tunable resonator. We show spectroscopy and Rabi oscillations of the qubits far detuned from the resonator. Data showing a relaxation time of 1μs and a Rabi time of 200 ns have so far been obtained.
8:12AM V17.00002 Superconducting qubits can be coupled and addressed as trapped ions\(^1\), Y.X. LIU, L.F. WEI, J.R. JOHANSSON, RIKEN, Japan, J.S. TSAI, RIKEN and NEC, Japan, F. NORI, RIKEN, Japan, and the Univ. of Michigan, Ann Arbor, USA — Exploiting the intrinsic nonlinearity of superconducting Josephson junctions, we propose a scalable circuit with superconducting qubits (SCQs) which is very similar to the successful one now being used for trapped ions. The SCQs are coupled to the “vibrational” mode provided by a superconducting LC circuit or its equivalent (e.g., a superconducting quantum interference device). Both single-qubit rotations and qubit-LC-circuit couplings and/or decouplings can be controlled by the frequencies of the time-dependent magnetic fluxes. The circuit is scalable since the qubit-qubit interactions, mediated by the LC circuit, can be selectively performed, and the information transfer can be realized in a controllable way. Y.X. Liu, L.F. Wei, J.R. Johansson, J.S. Tsai, F. Nori, Superconducting qubits can be coupled and addressed as trapped ions, Phys. Rev. B 76, 144518 (2007). URL: http://link.aps.org/abstract/PRB/v76/e144518

\(^1\)Supported in part by LPS, NSA, ARO, NSF, CREST, and RIKEN.

8:24AM V17.00003 Second order dispersive regime of circuit QED with a transmon qubit, MAXIME BOISSONNEAULT, Universite de Sherbrooke, J. M. GAMBITTA, IQC and University of Waterloo, ALEXANDRE BLAIS, Universite de Sherbrooke — In many recent circuit QED experiments, a transmon-type qubit is fabricated inside a high-Q transmission line resonator. Compared to the Cooper-pair box (CPB), the transmon has both a stronger coupling to the resonator and a significantly longer dephasing time. By going to the dispersive regime, where the qubit-resonator detuning is much larger than the coupling strength, the qubit can be controlled and measured through the resonator. In previous work, we have shown that one must include non-linear corrections to the dispersive approximation in strong measurements of a CPB qubit. These corrections cause a saturation of the signal-to-noise ratio and photon-dependant qubit decay and dephasing rates. In this talk, we will show how these non-linear corrections come into play with the transmon, and how they could be used to improve the measurement. [1] Houck et al, Nature, 2007, 449, 328 [2] Majer et al, Nature, 2007, 449, 443 [3] Koch et al, PRA, 2007, 76, 042319, [4] Schreier et al PRB 77, 180502 (2008), [5] Boissonneault et al, PRA, 2008, 77, 060305(R).

8:36AM V17.00004 Two Cavity Circuit QED, BLAKE JOHNSON, Yale University, ANDREW HOUCK, Princeton University, JAY GAMBITTA, University of Waterloo, ALEXANDRE BLAIS, University of Sherbrooke, STEVEN GIRVIN, MICHEL DEVORET, ROBERT S. SCHOELKOPF, Yale University, YALE CIRCUIT QED TEAM — The circuit QED architecture has proven useful for dispersive manipulation and measurement of superconducting qubits. Previous experiments have shown how to use the AC-Stark shift to spectroscopically extract information about the photon number in the cavity[1]. Here we will show how to extend this toward building a photon statistics analyzer by adding a second cavity to the circuit QED architecture. The second cavity allows for decoupling of the preparation and readout of the cavity field state, opening the way for a measurement of the full photon statistics and reconstruction of the Wigner distribution.


8:48AM V17.00005 Multi-Transmon circuit QED using local and fast flux biasing, LEONARDO DICARLO, JERRY CHOW, Yale University, JOHANNES MAJER, Vienna University of Technology, LUIGI FRUNZIO, Yale University, JAY GAMBITTA, University of Waterloo, ALEXANDRE BLAIS, Universite de Sherbrooke, STEVEN GIRVIN, ROBERT S. SCHOELKOPF, Yale University — We report local and fast flux tuning of Transmon qubits in circuit QED by means of proximal short-circuited coplanar waveguides. We characterize the effect of these additional microwave channels on qubit lifetime. We demonstrate one-qubit Z-gates and time-domain control of two-qubit interaction via virtual photon exchange. Gate performance is characterized by process tomography and compared to gating by AC Stark shift as previously investigated by the Yale CQED team [1]. Research supported by NSF, NSA and ARO. [1] Majer et al., Nature 449, 443 (2007).

9:00AM V17.00006 Inline Cavity Qubit with Bifurcation Readout, MARKUS BRINK, NICHOLAS A. MASLUK, KURTIS L. GEERINGS, Yale University, MICHAEL METCALFE, NIST Gaithersburg, VLADIMIR MANUCHARYAN, LUIGI FRUNZIO, STEVEN M. GIRVIN, ROBERT J. SCHOELKOPF, MICHEL H. DEVORET, Yale University — We present the design and data from a new, strongly coupled superconducting qubit based on Josephson junctions and a strictly 1-dimensional distributed element geometry that operates in the Transmon regime. A cavity bifurcation amplifier is used to read the state of the qubit. The same circuit also supports a linear dispersive readout, which enables direct comparison between the latching and dispersive scheme. Most recent results will be discussed.

9:12AM V17.00007 Generation of entangled states in circuit QED using sideband transitions, P.J. LEEK, S. FILIPP, P. MAURER, ETH Zurich, A. BLAIS, Universite de Sherbrooke, A. WALLRAFF, ETH Zurich, ETH QUANTUM DEVICE TEAM — The deterministic generation of entanglement between pairs of distant qubits is an important goal in the development of a quantum information processor. A promising and potentially scalable method of achieving this is through the use of sideband transitions between qubits and a globally coupled harmonic oscillator. Most recent results will be discussed.

9:24AM V17.00008 Generating entanglement by measurement in circuit QED, JAY GAMBITTA, CHANTAL HUTCHISON, University of Waterloo, ALEXANDRE BLAIS, Universite de Sherbrooke, FRANK WILHELM, University of Waterloo — In this talk, we will show theoretically how to induce entanglement by measurement in circuit QED. I will use quantum trajectory theory to derive an equation for the conditional state of a two qubit system, conditioned on continuous-in-time measurement of the amplitude and phase of the field leaving the resonator. I will show that with experimental parameters, we can have a decoherence-free subspace to generate an entangled state with a high concurrence and with a success probability of 1/2. Finally I will show that with a simple feedback scheme the same concurrence can be achieved with a success probability of one.

9:36AM V17.00009 Towards proving non-classicality with a 3-qubit GHZ state in circuit QED, LEV S. BISHOP, Yale University, JAY M. GAMBITTA, University of Waterloo, ERAN GINOSSAR, STEVEN M. GIRVIN, Yale University, ANDREW A. HOUCK, Princeton University, JENS KOCH, ANDREAS NUNENKAMP, DAVID J. PRICE, ROBERT J. SCHOELKOPF, Yale University, LARS TORNBERG, Chalmers University of Technology, YALE CIRCUIT QED TEAM — The demonstration of violation of Bell-type inequalities remains challenging for superconducting qubits, due to short coherence times and limited measurement fidelity. Here, we propose to utilize 3-qubit GHZ states in a circuit QED system to accomplish this key step. In contrast to other schemes where the qubits are measured individually, circuit QED offers the advantage that a single dispersive measurement can directly reveal the parity (\(\sigma_1 \otimes \sigma_2 \otimes \sigma_3\)). When combined with appropriate 1-qubit rotations, this provides the necessary ingredients to obtain an effective measurement of Mermin’s Bell operator with less stringent requirements on the measurement fidelity. Generation of the GHZ state can proceed via either 1- and 2-qubit gates or preparation by measurement. We present results from quantum trajectory calculations and estimate the resulting violation of the Mermin inequality, based on experimentally feasible parameters.
9:48AM V17.00010 Exploration of the Tavis-Cummings Model with Multiple Qubits in Circuit QED
J.M. Fink, ETH Zurich, A. Blais, Universite de Sherbrooke, A. Wallraff, ETH Zurich, ETH Quantum Device Team — Superconducting qubits in coplanar waveguide resonators provide an unprecedentedly large dipole coupling strength to microwave frequency photons confined in an on-chip waveguide resonator [1]. In contrast to atoms in traditional vacuum QED a controlled number of qubits remain at fixed positions with constant coupling to the cavity field at all times. Utilizing these properties we have performed measurements with up to three independently flux-tunable qubits to study cavity mediated multi-qubit interactions. By tuning the qubits in resonance with the cavity field individually, we demonstrate the square root of $N$ scaling of the collective dipole coupling strength with the number of resonant atoms $N$ as described by the Tavis-Cummings model. To our knowledge this is the first observation of this nonlinearity in a system in which the atom number can be changed one by one in a discrete fashion. In addition, the energies of both bright and dark coupled multi-qubit / photon states are well explained by the Tavis-Cummings model over a wide range of detunings. On resonance we obtain an equal superposition of a photon and a Dicke state with an excitation equally shared among the $N$ qubits.


10:00AM V17.00011 Two-photon probe of the Jaynes-Cummings model and controlled symmetry breaking in circuit QED, Frank Deppe, Matteo Mariantoni, E. P. Menzel, A. Marx, R. Gross, Walther-Meissner-Institut and TU Muenchen, Germany, S. Saito, K. Kakuyanagi, H. Tanaka, K. Semba, NTT Basic Research Laboratories, NTT Corp., Japan, T. Meno, NTT Advanced Technology, NTT Corp., Japan, H. Takayanagi, Tokyo University of Science and International Center for Materials Nanoelectronics, Japan, E. Solano, Universidad del Pais Vasco - Euskal Herriko Unibertsitatea, Spain — Superconducting qubits behave as artificial two-level atoms. Coupling them on-chip microwave resonators has given rise to the field of circuit quantum electrodynamics (QED). In this work, we report on the observation of key signatures of a two-photon driven Jaynes-Cummings model, which unveils the upconversion dynamics of a superconducting flux qubit coupled to an on-chip resonator. Our experiment and theoretical analysis show clear evidence for the coexistence of one- and two-photon driven level anticrossings of the qubit-resonator system. This results from the controlled symmetry breaking of the system Hamiltonian, causing parity to become a not well-defined property. Our study provides deep insight into the interplay of multiphoton processes and symmetries in a qubit-resonator system. We acknowledge support from SFB631, NIM, CREST-JST, JSPS-KAKENHI (18201018), MEXT-KAKENHI (18001002), EuroSQIP, and the Ikerbasque Foundation.

10:12AM V17.00012 Dynamics of dispersive single qubit read-out in circuit QED, R. Bianchetti, S. Filipp, A. Blais1, A. Wallraff, ETH Zurich, ETH Quantum Device Team — In a circuit quantum electrodynamics setup the qubit state is inferred from the response of the coupled qubit-cavity system to a microwave signal applied close to the cavity resonance. We experimentally investigate the frequency dependence of the response for both weak continuous and pulsed measurement signals. We find excellent agreement with theoretical predictions from a generalized Jaynes-Cummings model which includes dissipation and dephasing. The quantitative understanding of the system response is used to optimize the measurement frequency maximizing the signal-to-noise ratio. This allows for an accurate determination of the qubit excited state population from the measured field response.

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10:24AM V17.00013 Two-qubit tomography with joint dispersive read-out in circuit QED, S. Filipp, P. Maurer, P. J. Leek, ETH Zurich, A. Blais, Universite de Sherbrooke, A. Wallraff, ETH Zurich, ETH Quantum Device Team — Quantum state tomography is an important tool in quantum information science for complete characterization of multi-qubit states and their correlations. We demonstrate that for two superconducting qubits coupled to a common resonator mode a reconstruction of the full density matrix can be achieved by measuring the transmission through the resonator — without the need for single-shot measurement of individual qubits. Since the resonator transmission depends non-linearly on the dispersive cavity pull of different qubit states, information about qubit-qubit correlations is intrinsically present in the averaged measurement signal. It is shown that this simultaneous two-qubit read-out can be used for quantum state tomography of both separable and entangled states.

10:36AM V17.00014 Measurement of Autler-Townes and Mollow transitions in a strongly driven superconducting qubit, M. Baur, S. Filipp, ETH Zurich, A. Blais, Universite de Sherbrooke, A. Wallraff, ETH Zurich, ETH Quantum Device Team — The spectrum of a multilevel atom can be significantly modified when interacting with electromagnetic fields. In the simplest case where a two-level atom is driven on resonance, two sidebands offset from the main atomic line by the Rabi frequency Ω appear in the fluorescence spectrum, referred to as the Mollow triplet. Similarly, when probing transitions into a third atomic level, the absorption spectrum shows two spectral lines separated by Ω, called the Autler-Townes doublet. Here we present a measurement of the Autler-Townes doublet and the sidebands of the Mollow triplet in a strongly driven superconducting qubit. The corresponding transitions are detected using dispersive read-out of the qubit coupled off-resonantly to a microwave transmission line resonator. The observed frequencies of the Autler-Townes and Mollow spectral lines are in excellent agreement with a generalized dispersive Jaynes-Cummings model.

10:48AM V17.00015 Microwave Photon Detector in Circuit QED, Juan Jose Garcia-Ripoll, Instituto de Física Fundamental, CSIC, Guillermo Romero, Departamento de Fisica, Universidad de Santiago de Chile, Enrique Solano, Departamento de Quimica-Fisica, Universidad del Pais Vasco, Bilbao — In this work we propose a design for a microwave photodetector based on elements from circuit QED such as the ones used in qubit designs. Our proposal consists on a microwave guide in which we embed circuit elements that can absorb photons and irreversibly change state. These incoherent absorption processes constitute the measurement itself. We first model this design using a general master equation for the propagating photons and the absorbing elements. We find that the detection efficiency for a single absorber is limited to 50%, and that this efficiency can be quickly increased by adding more elements with a moderate separation, obtaining 80% and 90% for two and three absorbers. Our abstract design has at least one possible implementation in which the absorbers are current biased Josephson junction. We demonstrate that the coupling between the guide and the junctions is strong enough, irrespectively of the microwave guide size, and derive realistic parameters for high fidelity operation with current experiments. Patent pending No. 200802933, Oficina Espanola de Patentes y Marcas, 17/10/2008.
8:00AM V18.00001 Spectroscopic Analyses of Microstructures Associated with Plant Based Polymers

SHAW LING HSU, Polymer Science and Engineering Department, University of Massachusetts at Amherst — Currently, less than 0.02% of polymers used are plant based with the remaining 99.98% of polymers produced from petroleum. The use of plant based polymers can have a significant impact on the cost of the petroleum. Because of their size scale, it is most appropriate to use vibrational and NMR spectroscopy to characterize the microstructure of these plant based polymers. We present a number of examples in order to illustrate the use of these alternative polymers. Soybean is one of the most promising alternatives. Both its saturated and unsaturated components can be utilized. In various applications, the saturated component is important because the rapid crystallization directly controls the rheological behavior. This is especially significant if co-crystallization with other polymers, especially statistically random copolymers, is an important consideration. Crystallization kinetics and subsequent morphological units formed have yet to be characterized. In addition, the unsaturated component can be modified to form various polyols for use in reactive mixtures. The miscibility behavior of such polymers with other oligomers or polymers strongly influences the reaction kinetics and the products formed. The extreme hydrophobic nature of soybean based polymers is reflected in that it has a characteristic of poly(lactic acid). We have characterized the inherent structural rigidity, correlating the changes in chain conformation to the chain conformation. We have identified the intermolecular forces which stabilized the crystalline units. In addition, we have been able to control the crystallization process resulting from addition configurational defects. This presents an opportunity the we have available in a world which may embrace such a set of polymers.

8:36AM V18.00002 Toughening and reinforcing degradable polymers to extend their properties and applications

SUPING LYU, Medtronic Inc, JIANBIN ZHANG, ADAM BUCKALEW, JIM SCHLEY, BRYANT PUDIL, LIAN LUO, CHRIS HOBOT, MIKE BENZ, RANDY SPARER, JULIE TRUDEL — Polymer materials made from renewable feedstocks mainly are cellulose derivatives and aliphatic polyesters such as polylactide. There are two challenges in the use of these materials to replace petroleum based polymers. One is how to easily process these materials to make them into needed shapes and other is how to broaden the properties of these materials so that they can be used for applications where petroleum based polymers play major roles. Most of the renewable source based materials are brittle. This abstract presents a method of how to toughen and reinforce polylactide to make a family of polymers that cover broad ranges of toughness and strength for various applications such as biomedical device manufacturing.

8:48AM V18.00003 A QC-MD Study of the Enzymatic Degradation of Cellulose Thin Films

DAN GLICKMAN, OLEH TANCHAK, MICHAEL REID, AMANDA QUIRK, DARRELL COCKBURN, COLIN MACDOUGALL, ANTHONY CLARKE, JACEK LIPKOWSKI, JOHN DUTCHER, University of Guelph — A sophisticated surface-sensitive technique, the quartz crystal microbalance with dissipation monitoring (QC-MD), was used to study the interaction of a mixture of cellulolytic enzymes from the fungus T. reesei with cellulose thin films deposited onto polycrystalline gold surfaces. It was found that the amylolytic enzymes on the gold substrate led to two processes that occur during the enzyme mixture-cellulose thin film experiment: adsorption of the enzyme to the film surface, and the subsequent degradation of the cellulose thin film. A model describing the measured frequency shift in the QCM data will be described, which gives excellent fits to the experimental data.

9:00AM V18.00004 An Atomic Force Microscopy Study of the Mechanism of Cellulose Biodegradation

AMANDA QUIRK, MAOHUI CHEN, DARRELL COCKBURN, SARAH REGLI, ANTHONY CLARKE, JOHN DUTCHER, JACEK LIPKOWSKI, University of Guelph, SHARON ROSCOE, Acadia University — Cellulose, a biopolymer consisting of long chain β-(1→4) linked glucose sugars, is used as structural material by plants and bacteria. Degradation of cellulose to glucose, a sugar easily fermented to ethanol, occurs by the enzymatic hydrolysis of cellulose by cellulase enzymes. The enzymes have a complex structure including carbohydrate binding modules and catalytic domains responsible for the binding and degradation of cellulase, respectively. Atomic force microscopy (AFM) was used to study native cellulose films prepared from Acetobacter xylinum using a novel application of the Langmuir-Blodgett technique. These films allowed AFM images of single fibers and their microfibril structure to be obtained. Further in situ AFM studies of single fibers were performed in solution using cellulolytic enzymes. The in situ degradation of cellulose fibers was monitored over 20-hours using AFM. These studies provided insight into the degradation timeline of a single fiber. Complementary studies of proteins adsorbed on cellulose fibers revealed information about the binding of the enzymes to the substrate. Studying the modular enzyme action separately will provide insight into the mechanism of cellulose binding and contribute to our understanding of the degradation process.

9:12AM V18.00005 Observation of Biodegradation of Cellulose Fibers Using Surface Plasmon Resonance Imaging

OLEH M. TANCHAK, SCOTT ALLEN, Department of Physics, University of Guelph, DARRELL COCKBURN, ANTHONY J. CLARKE, Department of Molecular and Cellular Biology, University of Guelph, JACEK LIPKOWSKI, Department of Chemistry, University of Guelph, JOHN R. DUTCHER, Department of Physics, University of Guelph — Cellulose is the most abundant biopolymer on Earth and can provide a renewable supply of ethanol fuel to replace fossil fuels. A fundamental understanding of the mechanisms of the biodegradation of cellulose is essential to the development novel enzyme systems that can efficiently and selectively degrade a variety of biomass substrates. A novel Surface Plasmon Resonance Imaging (SPRI) instrument was used to study the biodegradation of cellulose fibers anchored to a titiated gold surface. The kinetics of binding of the inactive enzymes to cellulose fibers and their digestion by catalytically-active homologs will be presented.

9:24AM V18.00006 Sustainable Engineering and Improved Recycling of PET for High-Value Applications: Transforming Linear PET to Lightly Branched PET with a Novel, Scalable Process

CYNTHIA PIERRE, JOHN TORKELSON, Northwestern University — A major challenge for the most effective recycling of poly(ethylene terephthalate) concerns the fact that initial melt processing of PET into a product leads to substantial degradation of molecular weight. Thus, recycled PET has insufficient melt viscosity for reuse in high-value applications such as melt-blowing of PET bottles. Academic and industrial research has tried to remedy this situation by synthesis and use of “chain extenders” that can be added to branched PET (with higher melt viscosity than the linear recycled PET) via condensation reactions with functional groups on the PET. Here we show that simple processing of PET via solid-state shear pulverization (SSSP) leads to enhanced PET melt viscosity without need for chemical additives. We hypothesize that this branching results from low levels of chain scission accompanying SSSP, leading to formation of polystyrene radicals in the melt which then participate in condensation reactions with other PET chains and thereby to in situ branch formation. The pulverized PET exhibits vastly enhanced crystallization kinetics, eliminating the need to employ cold crystallization to achieve maximum PET crystallinity. Results of SSSP processing of PET will be compared to results obtained with poly(butylene terephthalate).

9:36AM V18.00007 Spontaneously Formed Biocompatible Surfaces in Water by Segregation of Amphiphilic Block Copolymers

HIDEAKI YOKOYAMA, The University of Tokyo, TAKASHI ISHIZONE, Tokyo Institute of Technology, NAOYA TORIKAI, High Energy Accelerator Research Organization, JAROSLAW MAJEWSKI, Los Alamos National Laboratory, AYAKO OYANE, AIST — Reduction of hydrophobic interaction in water is important in biological interfaces. We have found that poly(styrene-b-oligo ethylene glycol methyl ether methacrylate) (PS-PENMA) segregates the PENMA block to the surface in hydrophobic environment such as in air or in a vacuum, and shows remarkable resistance against adsorption or adhesion of proteins, platelets and cells in water. We studied the interfacial structures between PS modified by the spontaneous segregation of PS-PENMA and water using neutron reflectivity and adhesion force measurement using atomic force microscope with hydrophobic probes. The interfacial structure and hydrophobic interaction depend on the number of ethylene glycol (EO) units in PENMA. PENMAs with two or more EO units show distinct swollen layers with two sharp interfaces at polymer/water interfaces, which effectively reduce hydrophobic interaction in water, while PENMA with one unit of EO displays broader single interface with unsatisfactory reduction.
9:48AM V18.00008 Electros spun Nanofibers for Neural and Tissue Engineering, YOUNAN XIA, Washington University — Electros spinning has been exploited for almost one century to process polymers and other materials into nanofibers with controllable compositions, diameters, porosities, and porous structures for a variety of applications. Owing to its small size, high porosity, and large surface area, a nonwoven mat of electros spun nanofibers can serve as an ideal scaffold to mimic the extracellular matrix for cell attachment and nutrient transportation. The nanofiber itself can also be functionalized through encapsulation or attachment of bioactive species such as extracellular matrix proteins, enzymes, and growth factors. In addition, the nanofibers can be further assembled into a variety of arrays or architectures by manipulating their alignment, stacking, or folding. All these attributes make electros spinning a powerful tool for generating Nanostructured materials for a range of biomedical applications that include controlled release, drug delivery, and tissue engineering. This talk will focus on the use of electros spun nanofibers as scaffolds for neural and bone tissue engineering.

10:24AM V18.00009 Control of Protein Adsorption on Surfaces with Grafted Polymers, IGAL SZLEIFFER, Northwestern University, JAN GENZER, North Carolina State University — Non-specific protein adsorption is the first process in the foreign body response. The molecular design of surface modifiers that prevent non-specific adsorption requires the understanding of the factors that determine protein adsorption. The hierarchy of time and length scales present in the adsorption requires a multiscale approach to treat the complexity of the process. We will discuss the driving forces that determine protein adsorption and how end-grafted polymers can be used to modify the ability of the proteins to reach the surface. We will show the differences between preventing protein adsorption thermodynamically and kinetically. For practical applications the relevant time scales are hours or days. We will show how a molecular approach can be used to study these time scales. In particular we will show two different levels of approximations based on a molecular understanding of the adsorption process that enables, through the proper integration of degrees of freedom, to determine the kinetics of adsorption over 16 orders of magnitude in time. This approach is applied to explain recent experimental observations carried out on orthogonal modified surfaces that suggest that protein adsorption is a universal function of the product of grafted polymer surface coverage and molecular weight.

10:36AM V18.00010 Optimization of Polymer Surfaces for Specific Targeting2, ELENA DORMIDON-TOVA, MATTHEW HAGY, SHIHU WANG, Department of Macromolecular Science and Engineering, Case Western Reserve University — Using Monte Carlo simulations we studied reversible binding between a polymer layer functionalized by ligands and a receptor surface. By analyzing distance-dependent profiles for the average number of ligands bound to receptors, the total free energy of polymer layer-cell surface interaction and the interaction force the influence of different design parameters of a polymer layer on the affinity and specificity of binding were investigated. We show that planar polymer layers with a smaller chain length and grafting density, larger degree of functionalization, and larger absolute binding energy exhibit higher affinity to the cell surfaces with a large density of mobile receptors. A high binding specificity can be achieved by the polymer layers with intermediate ligand-receptor binding energies or an intermediate number of ligands, as a larger binding energy or number of ligands lacks specificity while a smaller binding energy or number of ligands provides inadequate affinity. As a result, the optimal design of the polymer layers can be achieved by using several different strategies, which will be discussed.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V19 DPOLY: Focus Session: Hierarchically Ordered Systems

8:00AM V19.00001 Semi-crystalline PMMA Stereocomplex Fibers, MATIJA CRNE, School of Chemistry and Biochemistry, Georgia Institute of Technology, SHIN-WOONG KANG, Department of Physics, Kent State University, JUNG OK PARK, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology, SATYENDRA KUMAR, Department of Physics, Kent State University, MOHAN SRINIVASARAO, School of Polymer, Textile and Fiber Engineering, Georgia Institute of Technology — A mixture of isotactic and syndiotactic PMMA polymers forms a supramolecular helical structure, called "stereocomplex" PMMA, which is held together by non-covalent bonding. The helices can pack together, resulting in a semi-crystalline material with a melting point of 172°C. Furthermore, the solutions exhibit gelation behavior in appropriate solvents. We have utilized these properties to make oriented stereocomplex PMMA fibers by three different methods — wet spinning, gel spinning and electrospinning. These fibers are highly oriented and crystalline. They are resistant to high temperatures up to 160°C. They are also resistant to the PMMA polymerization conditions. We have examined the fibers using X-ray diffraction and Raman spectroscopy. The results agree with the recently proposed triple helical structure where two isotactic PMMA chains wrap around each other in a double helix and then the syndiotactic chain wraps around this double helix. The resulting structure is a triple helix with a 1:2 molar ratio of isotactic : syndiotactic PMMA.

8:12AM V19.00002 Hierarchically Organized Pyrolyzed Core-Silica Shell Hybrids, AYSEGUL ALTUNBAS, NIKHIL SHARMA, DARRIN J. POCHAN, University of Delaware, Department of Materials Science & Engineering, JOEL P. SCHNEIDER, UNIVERSITY OF DELAWARE, DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY COLLABORATION — A biomimetic approach was applied for the fabrication of a 3D hybrid network that displays hierarchical organization of an inorganic layer around an organic self-assembled peptide fibril template. The 20 amino acid peptide used in this study consisted of alternating hydrophilic (lysine) and hydrophobic (valine) residues flanking a four amino acid turn sequence in the center. After intramolecular folding into a beta-hairpin conformation on addition of a desired solution stimulus, this peptide self-sembles into a 3D network of entangled fibrils rich in beta-sheet with a high density of lysine groups exposed on the fibril-surfaces. The lysine-rich surface chemistry was utilized to create a silica shell around the fibrils. The mineralization process of the fibrils was initiated under physiological conditions by adding the silica precursor, tetramethyl orthosilicate, to the pre-assembled hydrogel, which results in a porous silica network that retains the mesoscale structure of the peptide fibril network. Structural characterization via Transmission Electron Microscopy, cryogenic-Scanning Electron Microscopy, Small Angle Neutron and X-ray Scattering and mechanical characterization via oscillatory rheology will be presented.

2This work was supported by the NIH grant R21CA112436

2Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China

8:12AM V19.00002 Hierarchically Organized Pyrolyzed Core-Silica Shell Hybrids, AYSEGUL ALTUNBAS, NIKHIL SHARMA, DARRIN J. POCHAN, University of Delaware, Department of Materials Science & Engineering, JOEL P. SCHNEIDER, UNIVERSITY OF DELAWARE, DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY COLLABORATION — A biomimetic approach was applied for the fabrication of a 3D hybrid network that displays hierarchical organization of an inorganic layer around an organic self-assembled peptide fibril template. The 20 amino acid peptide used in this study consisted of alternating hydrophilic (lysine) and hydrophobic (valine) residues flanking a four amino acid turn sequence in the center. After intramolecular folding into a beta-hairpin conformation on addition of a desired solution stimulus, this peptide self-sembles into a 3D network of entangled fibrils rich in beta-sheet with a high density of lysine groups exposed on the fibril-surfaces. The lysine-rich surface chemistry was utilized to create a silica shell around the fibrils. The mineralization process of the fibrils was initiated under physiological conditions by adding the silica precursor, tetramethyl orthosilicate, to the pre-assembled hydrogel, which results in a porous silica network that retains the mesoscale structure of the peptide fibril network. Structural characterization via Transmission Electron Microscopy, cryogenic-Scanning Electron Microscopy, Small Angle Neutron and X-ray Scattering and mechanical characterization via oscillatory rheology will be presented.
8:24AM V19.00003 Hierarchically Structured Regioregular Conjugated Polymer via Evaporative Self-Assembly

MYUNGHWAN BYUN, ROBYN LASKOWSKI, Iowa State University, FENG QIU, The Key Laboratory of Molecular Engineering of Polymers at Fudan University, Shanghai, China. We acknowledge the supports from NSF (CBET-0730611), 3M, and the Key Laboratory of Molecular Engineering of Polymers at Fudan University, Ministry of Education, China.

8:36AM V19.00004 Combining Small Molecule with Block Copolymer: a Facile Approach to Direct Hierarchical Assembly of Nanoparticles

TING XU, University of California, Berkeley — Precise control over the spatial organization of nanoscopic building blocks over multiple length scales is a bottleneck in the “bottom-up” approach to generate technologically important materials. We demonstrate a new paradigm to control the hierarchical assembly of nanoparticles through the synergistic co-assembly of block copolymers (BCP), small molecules and readily available nanoparticles. Organizations of nanoparticles into one, two and three-dimensional arrays with controlled inter-particle separation and ordering were achieved without any chemical modification of the BCPs, the order and distribution of small molecules within the BCPs are temperature dependent. These efforts have involved developing new synthetic techniques. The hierarchical structure was fabricated from a volume of material by combining holographic patterning (HP) and block copolymer (BCP) self-assembly. The structure of the BCP was investigated as a function of the BCP architecture, BCP concentration and crystallization temperature. Upon heating the BCP, a non-monotonic change in the structure of the BCP occurred; on cooling the reverse occurs reflecting the dynamic change in the hierarchical structure. Transmission electron microscopy, in-situ FTIR and optical spectroscopy were used to correlate the optical property change with BCP/HPC morphology. This approach could open a gateway to fabricating multifunctional hierarchical nanostructured materials.

9:12AM V19.00005 Hierarchical volume gratings by combining holographic-patterning and block copolymer self-assembly

MICHAEL BIRKRANT, RUSSELL MARRON, CHRISTOPHER LI, Department of Material Science & Engineering, Drexel University, Philadelphia, PA; LALGUIDI NATARAJAN, VINCENT TONDIGLIA, TIMOTHY BUNNING, Materials Manufacturing Directorate, Wright-Patterson Airforce Base, OH — A novel hierarchical photonic crystal (HPC) was fabricated by combining top-down and bottom-up nanomanufacturing techniques. The hierarchical structure was fabricated from a volume of material by combining holographic patterning (HP) and block copolymer (BCP) self-assembly. The structure of the HPC was investigated as a function of the BCP architecture, BCP concentration and crystallization temperature. Upon heating the photonic crystal a red shift in the reflected wavelength occurs; but, an initial decrease in diffraction efficiency (DE) followed by an increase in DE indicates a non-monotonic change in the structure of the HPC. Upon cooling the reverse occurs reflecting the dynamic change in the hierarchical structure. Transmission electron microscopy, in-situ FTIR and optical spectroscopy were used to correlate the optical property change with BCP/HPC morphology. This approach could open a gateway to fabricating multifunctional hierarchical nanostructured materials.

9:24AM V19.00006 Heteroarm Star Block Copolyampholytes as Templates for Hierarchically-Ordered Polyelectrolyte-Surfactant Complexes

MATTHEW HAMMOND, CHAOXU LI, Univ. of Fribourg, Switzerland, CONSTANTINOS TSITSIKLISIANS, Univ. of Patras, Greece, RAFFAELE MEZZENGA, Univ. of Fribourg, Switzerland — We report on the hierarchical ordering observed in dry, solid samples of polyelectrolyte-surfactant complexes based upon a novel heteroarm star block terpolymer bearing short polystyrene (PS) arms and an equal number of longer poly(2-vinylpyridine)-block-poly(acrylic acid) (P2VP-b-PA) arms. The amphoteric nature of the star block copolymer allowed for complexation to be carried out on either the P2VP blocks (with negatively charged surfactants) or on the PA blocks (with positively charged surfactants), depending only on the pH at which the complexation reaction was carried out. X-ray scattering and transmission electron microscopy data reveal that the various complexes display self-organization on the length scale of the polyelectrolyte-surfactant complex (ca. 3 - 4 nm) and on that of the overall copolymer (ca. 20 - 40 nm), with the specific repeat distances and self-organized morphologies being dramatically affected by the choice of block to be complexed. This study clearly illustrates how topological design possibilities in hierarchical self-assembly of block copolymer-based supramolecular complexes can be greatly enhanced by increasing the level of complexity of the macromolecular templates used.

9:36AM V19.00007 Assembly of Organic/Nanoparticle Hybrid Systems

STEPHEN Z.D. CHENG, University of Akron, YINGFENG TU, CHUN YE, WENBINS CHANG, XINFEI YU, RYAN M. VAN HORN, CHIEN-LUNG WANG — The structure, dispersion, and chemical functionality of particles in a material are critical to the material’s properties. We are working to build the scientific and technological foundations of using particles such as C60 and POSS to develop new, highly functional, self-assembled materials. These efforts have involved developing new synthetic techniques to efficiently and precisely manipulate particles to control their dispersion and structure within the organic material. First, C60-polymer and POSS-polymer molecules have been synthesized. These materials are capable of crystallizing in solution, enabling the formation of highly conducting or insulating sheets on the basal surfaces of the crystals. Additionally, these molecules may form micelles in solution. Next, POSS-C60-porphyrin molecules were synthesized and were found to self-assemble into discotic columnar structures where the intimately arranged porphyrin core harvests photons and the C60 enhances charge transport, making these materials ideal for organic photovoltaic applications. Finally, C60-POSS conjugate molecules have been synthesized that crystallize into a bilayer organization of nanoscopic building blocks over multiple length scales, where the intimately arranged porphyrin core harvests photons and the C60 enhances charge transport.

9:48AM V19.00008 Quantification of the Molecular Topology for Hierarchical Macromolecules

GREGORY BEAUCAGE, University of Cincinnati — Hierarchical structures are often produced from ramified macromolecules such as comb, star, hyperbranched and dendritic polymers. We have recently derived a method for the description of complex molecular and nanostructural topologies based on a statistical analysis [1,2]. The method has been applied to a wide range of hierarchical materials from long chain branched polyolefins, hyperbranched polymers [3], star polymers, H-branched polymers to cyclcics, biopolymers [4], and branched nanostructured aggregates. This method, when applied to neutron scattering data, yields the molecular fraction of a structure involved in branching, the number of branch sites, the average branch length, and the number if inner chain segments. Further, quantitative measures of the tortuosity or connectivity of the structure and the connectivity of the branching network can be made, opening a new window for our understanding of complex molecular topologies. This understanding has recently been applied to biological chain molecules to understand protein and RNA folding [4] for example as well as to aggregated, nanostructured, carbon soot.

Glass Transition in Thin Supported Polymer Films


The observation of finally smooth ultra-thin regenerated cellulose fibers were obtained under high relative humidity. The water vapor played an important role in leading to "skin formation" which helped to stabilize the fibrous morphology, and chloride (AMIMCl) was investigated. It was found that the introduction of co-solvent dimethyl sulfoxide (DMSO) contributed to a continuous jet. The problems alter glass transition temperature assignment will be discussed. Residual gas can affect data even at the pressures mentioned above [1]. An ionization gauge, both linear and modulated temperature scans [1, 2]. A well-defined glass transition in 5 nm thick PS and 10 nm thick PMMA films is observed. Factors that can decrease the bead density that appears in the electrospun microfiber mat. Scanning and transmission electron microscopies are used to investigate both the surface and internal morphology of these fibers, along with the robustness of the micelles. The combination of self-assembled structures within a polymer matrix can lead to fascinating response behavior dependent on temperature; if the sample is heated and the melting point of PFS is surpassed, the micelles will melt upon electrospinning.

The PFS-P2VP homopolymer solution and electrospun. Addition of the cylindrical micelles is found to improve the ability of P2VP to be electrospun and dramatically develop in dimethylformamide (DMF), a P2VP-selective solvent, with lengths exceeding one micron. These self-assembled micelles are then incorporated into P2VP homopolymer solution and electrospun. Addition of the cylindrical micelles is found to improve the ability of P2VP to be electrospun and dramatically decrease the bead density that appears in the electrospun microfiber mat. Scanning and transmission electron microscopies are used to investigate both the surface and internal morphology of these fibers, along with the robustness of the micelles. The combination of self-assembled structures within a polymer matrix can lead to fascinating response behavior dependent on temperature; if the sample is heated and the melting point of PFS is surpassed, the micelles will melt and then form classical morphologies. In the case of self-assembled, conductive cylinders of PFS block copolymers, heating the sample destroys conductive pathways. The PFS-P2VP self-assembled cylinders have also been incorporated into other DMF-selective polymers to verify that the micelles remain intact upon electrospinning.

Electrospinning of native cellulose from nonvolatile solvent system. SHAN-SHAN XU, AIHUA HE, CHARLES C. HAN, Institute of Chemistry, CAS — Electrospinning of cellulose in a highly efficient RTIL of 1-allyl-3-methylimidazolium chloride (AMIMCl) was investigated. It was found that the introduction of co-solvent dimethyl sulfoxide (DMSO) contributed to a continuous jet. The problems lying in nonvolatility and the high ionic strength of the RTIL were successfully resolved using a rotating copper-wire drum as a collector and solidifying the jet under high relative humidity. The water vapor played an important role in leading to “skin formation” which helped to stabilize the fibrous morphology, and finally smooth ultra-thin regenerated cellulose fibers were obtained.

Thursday, March 19, 2009 8:00AM - 11:00AM
Session V20 DPOLY: Thin Films and Adhesion II

Electrospinning of native cellulose from nonvolatile solvent system.

Electrospinning of native cellulose from nonvolatile solvent system.

Electrospinning of native cellulose from nonvolatile solvent system.

Electrospinning of native cellulose from nonvolatile solvent system.

Electrospinning of native cellulose from nonvolatile solvent system.
8:24AM V20.00003 Physical Aging in Nanoconfined Polymer Films: Importance of 3D vs. 1D Thermal Contraction in the Resulting Physical Aging Response. CONNIE B. ROTH, ELIZABETH A. BAKER, Dept. of Physics, Emory University, Atlanta, GA 30322, PERLA RITTIGSTEIN, JOHN M. TORKELSON, Dept. of Chemical & Biological Eng., Dept. of Materials Science & Eng., Northwestern University, Evanston, IL 60208 — Studies of physical aging in confined geometries have reported conflicting observations of changes in physical aging rates with decreasing film thickness. Accelerated physical aging with decreasing film thickness has been observed with gas permeation and ellipsometry in stiff backbone, so-called “high free volume,” polymers traditionally used in gas separation membranes. In contrast, no change or suppressed physical aging has been observed with fluorescence in flexible carbon-carbon backbone polymers. We have developed a new streamlined ellipsometry procedure that allows us to relatively quickly (~6 hrs) evaluate the physical aging characteristics of both stiff and flexible backbone polymers in a thin film geometry. We present measurements of physical aging rates using our new approach and compare these to existing results in the research literature. In addition, we also address the importance of 3D vs. 1D thermal contraction in the resulting physical aging response, which we believe is one of the key factors accounting for the observed qualitative differences in physical aging rate upon confinement from the existing studies.

8:36AM V20.00004 Segmental dynamics of supported and freestanding polystyrene thin films probed by dye reorientation. KEEWOOK PAENG, HAU-NAN LEE, STEPHEN SWALLEN, MARK EDGER, University of Wisconsin-Madison — The dynamics of both freestanding and supported polystyrene thick films (down to 15 nm) were studied by measuring the reorientation of dye molecules. Well below Tg, dye molecules were photobleached using intense linearly polarized light creating an anisotropic distribution. The anisotropy decay was measured using circularly polarized light and probing fluorescence parallel and perpendicular to the bleaching beam during linear temperature ramping. Temperature ramping anisotropy measurements allow us to compare both dynamics and the distribution of relaxation times in thin and thick films. Both freestanding and supported thin films show faster and more broadly distributed dynamics than thick films. For 17.5 nm supported films, temperature ramping experiments show up to 14K shift in dynamics. The corresponding shift for 16.5nm freestanding films was 22K.

8:48AM V20.00005 Modeling Dielectric Relaxation in Simulations of Polymer Glasses and Thin Films. HENDRIK MEYER, Institut Charles Sadron, CNRS UPR22, Strasbourg, France, SIMONE PETER, J. BASCHNAGEL — We perform molecular dynamics simulations to study the dielectric relaxation of a bead-spring model for a polymer melt in the bulk and in supported films [1]. By assigning dipole moments parallel and perpendicular to the backbone of all chains in the completed simulation trajectories we calculate the dielectric spectra of so-called type-A polymers which exhibit relaxation processes due to the local motion of chain segments (“segmental mode”) and due to fluctuations of the end-to-end vector (“normal mode”). We find that the relaxation of both modes is enhanced in the films relative to the bulk. For the segmental mode this difference between film and bulk dynamics increases on cooling toward the glass transition. By a layer-resolved analysis of the segmental relaxation we show that the acceleration of the average film dynamics is a consequence of a smooth gradient in relaxation, originating from both interfaces where the segmental dipoles relax much faster than in the bulk.


9:00AM V20.00006 Neighboring Domains Perturb Glass Transition Temperature on Multilayer Films and Nanostructured Polymer Blend Systems. SOYOUNG KIM, CONNIE ROTH, RODNEY PRIESTLEY, JOHN TORKELSON, Northwestern University — The impact of free surface and polymer-substrate interfaces on the glass transition temperature (Tg) in nanoconfined geometries has been studied for over a decade. Free surfaces reduce the requirement for cooperative dynamics and tend to decrease Tg; attractive interactions with a substrate interface reduce mobility and tend to increase Tg. Employing a multilayer fluorescence technique, we show how the Tg dynamics of PS layers are perturbed by immiscible polymer-polymer interfaces. We determine the length scale over which adjoining layers can perturb the PS layer. Finally, we demonstrate the tunability of the Tg of ultrathin PS layers atop different types of polymers. Our results indicate that the cooperative segmental dynamics of an ultrathin PS layer are strongly coupled to the neighboring domains through the narrow polymer-polymer interface. These results suggest a novel route to create new material properties controlled by the type and thickness of polymers in a multilayer film geometry. Studies with nanostructured blends to monitor Tg perturbation by neighboring domain are also underway.

9:12AM V20.00007 Near Surface Dynamics of Polymers Probed with Nanoparticle Embedding. DONGPING QI, JAMES A. FORREST, Dept. of Physics and Astronomy, University of Waterloo — We use nanoparticle embedding to probe the dynamics of the near surface layer of glassy polymer films. We observe evidence for heterogeneous dynamics in the first 5-10 nm near the free surface of glassy polymers. We observe that the relaxation into the polymer immediately below the free surface is irreversible, even after a period of 1 year. On the other hand, further embedding (5-10 nm) appears to be reversible. The results are discussed in terms of possible models of near surface mechanical properties.

9:24AM V20.00008 Glass Transition of Thin Star Polymer Films. EMMANOUIL GLYNOS, University of Michigan, Ann Arbor, PETER GREEN, University of Michigan — The thickness dependence of the glass transition, Tg, of thin film polystyrene (PS) star molecules, supported by SiO2 substrates, has been examined using spectroscopic ellipsometry and compared to the behavior of linear PS chains. Linear PS chains exhibit a film thickness dependence on SiO2 substrates, decreasing with decreasing film thickness, for thicknesses h less than approximately 45 nm. This thickness dependence, when normalized by the bulk Tg, is observed for chains with a wide range of degrees of polymerization N, from N < Nc. (molecular weight between entanglements) to very large values of N. The Tg's of long chain star molecules, of low functionalities, f, exhibit the same thickness dependence. However, as the degree of polymerization of an arm length, Na, decreases the thickness dependence undergoes a transition, wherein Tg increases with decreasing h. These effects are discussed in terms of the role of architecture and entropic effects on the structure of the system. Implications on the chain dynamics will also be discussed.

9:36AM V20.00009 The Glass Transition in Ultra-Thin Polymer Films Confined between Structured Surfaces. VIJKRAM KUPPA, University of Cincinnati, GREGORY RUTLEDGE, MIT — Molecular Dynamics simulations are used to probe the structure and dynamics of polymers in ultra-thin slit pores. The simulation setup follows the structure of polymer nanocomposites, depicting chains intercalated between layered inorganic silicates. The structure and dynamics of bead-spring oligomers are studied for different film thicknesses, surface-segment interactions and temperature. In particular, we focus on the glass transition of the confined films as a function of layer thickness, interaction strength and density profiles: Tg is demonstrated to increase with confinement and attraction of the polymer with adjacent surfaces. The fragility of the polymer glasses is drastically different from the corresponding bulk system, and is shown to be dependent on the effective co-ordination number.

9:48AM V20.00010 Apparent changes in the molecular dynamics of thin polymer layers due to the impact of interfacial layers. ANATOLI SERGHEI, University of Massachusetts Amherst, MARTIN TRESS, FRIEDRICH KREMER, University of Leipzig, Germany — Possible mechanisms leading to an apparent faster glassy dynamics in thin polymer layers, as investigated by means of Broadband Dielectric Spectroscopy, are analyzed in detail. It is shown that manifold experimental findings can be traced back to the influence of interfacial sub-layers, where — due to the proximity to solid interfaces — the dielectric function of the polymer is altered and modifies, by that, the overall dielectric response of the polymer films. A large amount of experimental data is analyzed to evidence how the contribution of the interfacial dynamics combines with that of the bulk in order to give the total response of a thin polymer film. It is shown that the non-linear character of this combination could lead to apparently discrepant experimental results.
10:00AM V20.00011 Post-confinement Relaxation Behavior of Nanostructures on Polymer Surface

SHANHONG XU, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University — Dimensional relaxation of nanostructures on polymer film was studied to understand dynamics at surfaces and post-confinement relaxation. Line gratings from 33 nm and up on PS surface were formed by nanoimprint lithography, and AFM was used to monitor their relaxation with time and temperature. When annealed at temperatures in the vicinity of the bulk Tg, the grating height slumps – or shrinks – as surface tension and other driving forces overcome the viscosity. The temperature for rapid slumping decreases at smaller and smaller gratings of all molecular weights, but a simple explanation based on enhanced surface mobility due to increased surface to volume ratio fails to explain the results. Analysis of viscosity shows that the stress from surface tension may cause shear thinning and thus contribute to the reduced nanostructure stability. More importantly, confinement of polymer chains to spatial dimensions comparable to or even smaller than the radius of gyration seems to enhance molecular relaxation, which may be the major factor for the surprisingly low slumping temperature.

1Acknowledgement goes to NSF (CMMI-0728352) and Zeiss Excellence Center at UC Irvine.

10:12AM V20.00012 Molecular weight and chain architecture dependence of glassy compliance of ultrathin freely standing polymer films

SHANHONG XU, GREGORY B. MCKENNA, Texas Tech University — Glassy compliance of ultrathin linear polystyrene of different molecular weights was investigated with the novel nanobubble inflation techniques developed in our lab. Previous work by O’Connell, Hutcheson and McKenna [1] indicates that the glassy compliance decreases as the film thickness decreases for a polystyrene sample with molecular weight of 1M g/mol. However the glassy stiffening is not nearly as dramatic as that observed in the rubbery plateau regime [2]. Preliminary results in the present work show that the glassy compliance decreases as the molecular weight increases. We are now examining a three-arm star polystyrene with branch molecular weight the same as that of the lower molecular weight linear material and eight-arm stars will also be investigated with the purpose of determining chain architecture effects on the glassy and rubbery behaviors of ultrathin polymer films.


1contact author

10:24AM V20.00013 Surface Chemistry Effects on the Reactivity and Properties of Nanoconfined Bisphenol M Dicyanate Ester in Controlled Pore Glass

SHANHONG XU, GREGORY B. MCKENNA, Department of Chemical Engineering, Texas Tech University — The influence of nanoconfinement on the cure kinetics and glass transition temperature of a bisphenol M dicyanate ester/polycyanurate material is investigated as a function of surface chemistry and nanoconfinement size in controlled pore glass (CPG). The glass transition temperature and conversion as a function of cure time is investigated using differential scanning calorimetry. The native CPG surface accelerates the cure of bisphenol M dicyanate to a larger extent compared to the silanized hydrophobic CPG presumably because of the catalytic nature of surface hydroxyl groups of the native pores.

The length scale associated with the secondary Tg is depressed by 60 K at 11.5 nm, and the secondary Tg is 10 to 33 K above the primary Tg. The length scale associated with the secondary Tg is approximately 0.8 nm. Based on the measurements of both Tg and sol content as a function of conversion, the network structure does not change upon nanoconfinement.


1We acknowledge the American Chemical Society Petroleum Research Fund Grant 45416-AC7

10:36AM V20.00014 Relation Between Glass Transition Temperatures in Polymer Nanocomposites and Polymer Thin Films

JAMIE KROPKA, SANDIA NATIONAL LABORATORIES, VICTOR PRYAMITSYN, VENKAT GANESAN, Texas A&M University — Motivated by recent experiments, we examine within a percolation model whether there is a quantitative equivalence in the glass transition temperatures of polymer thin films and polymer nanocomposites (PNCs). Our results indicate that while the qualitative behaviors of these systems are similar, a quantitative equivalence cannot be established in general. However, we propose a phenomenological scaling collapse of our results which suggests a simple framework by which the results of the thin films may be used to quantitatively predict the properties of PNCs. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.

10:48AM V20.00015 Finite Element Analysis of Nanoparticle embedding into glassy polymers

MARK ILTON, JAMES A. FORREST, Dept. of Physics and Astronomy, University of Waterloo — The embedding of rigid nanospheres into the surface of thin film glassy polymers was modelled using a Finite Element Analysis. This method of analysis readily adapts to various material models, film thicknesses, and substrates. Moreover, it allows for modelling of the related hole relaxation process when embedded nanospheres are removed from the film. Calculations using a viscoelastic constitutive model with depth dependent material properties are compared to recent experimental results. The results are discussed in the context of the proposed near surface enhanced dynamics in thin film glassy polymers.
8:12AM V21.00002 Crystal orientation control of CdTe epitaxial layers grown on (100) GaAs with ZnSe buffer layer by molecular beam epitaxy¹, QIANG ZHANG, WILLIAM CHARLES, BINGSHENG LI, AIDONG SHEN, CARLOS MERILES, MARIA TAMARGO, The City College of the City University of New York — Based on our previous experience with the growth of ZnSe on GaAs, we have improved the substrate, on which we deposit CdTe by first depositing a ZnSe buffer on the bulk GaAs crystals. This allows us to control the I-V/III-V heterovatent epitaxy prior to the CdTe deposition. Depending on the control of the interface between ZnSe and CdTe, it was possible to stabilize the growth of either (100) or (111) CdTe epitaxial layers on the (100) ZnSe/GaAs substrate. Reflection high-energy electron diffraction was used to observe the nucleation of the epitaxial layers in situ during the growth, while x-ray diffraction and photoluminescence measurements indicate that the CdTe is of high structural quality despite the large lattice constant mismatch of 14.3% between CdTe and ZnSe. To explore the full impact of controllable-orientation growth technique, optical pumping and time-resolved Faraday rotation experiments were performed on CdTe films grown in different crystal orientation.

¹ NSF-NIRT Grant No. ECS-0608763

8:24AM V21.00003 Development of a Wafer Fusion Process for Producing Patterned GaP Templates, KRONGTIP TERMKOAA, VAIBHAV MATHUR, XIFENG QIAN, WILLIAM GOODHUE, Photonics Center, Dept. of Physics and Applied Physics, University of Massachusetts Lowell, DAVID BLISS, Air Force Research Laboratory/RWLA, Hanscom AFB, RITA PETERSON, Air Force Research Laboratory/RYJW. Wright-Patterson AFB — Quasi-phase-matching (QPM) is an effective technique for nonlinear optical frequency conversion to generate IR wavelengths not readily available from direct laser sources. The QPM gratings can be produced by electric field poling in ferroelectric oxide materials, or by crystal growth of alternating phase domains in the case of semiconductors. For semiconductor materials GaAs and GaP we are developing new patterning methods to produce optical gratings for QPM. The state of the art for producing orientation-patterned GaAs material is already well developed. Gallium phosphide (GaP), also transparent at IR wavelengths, is attracting interest for nonlinear optical frequency conversion due to its high second-order nonlinear susceptibility, high thermal conductivity, wide band gap and low optical loss. Here we report a method to fabricate a GaP periodic domain inversion template using a process combining wafer fusion, substrate removal, lithographic patterning, and wet/dry etching.

8:36AM V21.00004 Growth of GaN from Ga:In and Ga:Si liquid alloys¹, KATHLEEN KASH, CHALLA BEKELE, JOHN ANGUS, Case Western Reserve University — We grew GaN from Ga:Sn and Ga:In melt solutions that varied in composition from pure Ga to a few at.% Ga. Growth was done at 900 °C and 100 mtorr pressure by exposing the melt surface to a nitrogen plasma. A fit to a model of growth rate versus melt composition yielded estimates of the reaction rates for the formation of GaN versus composition of the melt that were, within experimental uncertainty, independent of the choice of diluents. Near-band-edge emission features were prominent in the photoluminescence spectra at both room temperature and 10 K for material grown from the entire range of melt compositions for both diluents. Lattice parameters measured by powder x-ray diffraction spectroscopy revealed an interesting dependence on melt composition; the “a” lattice parameter varied by as much as 1% and exhibited a minimum for material grown from melts with compositions between 60 and 70 at% Ga, for both diluents. One motivation for this work is growth of large area, high quality single crystal substrates.

¹This effort was funded in part by NSF DMR #9901419 and NSF DMR #0420765.

8:48AM V21.00005 Epitaxial Growth and Characterization of Void-Free 3C-SiC Films on Germanium-Modified Si Substrates using RTCVD, DOMINGO FERRER, SHAGANDEEP KAUR, SAYAN Saha, SEYOUNG KIM, EMANUEL TUTUC, SANJAY BANERJEE, Microelectronics Research Center, The University of Texas at Austin, NILRATAN MAZUMDER, Department of Applied Physics, IERCEM Institute of Information Technology (WBUT) — Cubic silicon carbide (3C-SiC) is an attractive wide band gap semiconductor, frequently employed under extreme conditions such as high temperature, high frequency and high power, due to its superior physical and chemical properties. The electronic properties of epitaxial graphene grown on SiC integrated on silicon substrates also offer great potential as a viable candidate for “beyond CMOS” devices. A detailed understanding of both the structure and growth of epitaxial graphene, and the SiC/Si interfaces is very important for designing feasible devices. To this end, the work will analyze the growth and characterization of 3C-SiC on Si(100) and Si(111) substrates. 3C–SiC epitaxial crystal growth was carried out at temperatures as low as 750°C using Rapid Thermal CVD. A thin germanium buffer layer was deposited on Si substrates prior to epitaxial growth of SiC to suppress the formation of voids. The precursors utilized were (CH3)3SiH and GeH4, for silicon carbide and germanium deposition, respectively.

9:00AM V21.00006 The role of strontium in oxide epitaxy on silicon (001), JAMES REINER, KEVIN GARRITY, FRED WALKER, SOHRAIB ISMAIL-BEIGI, CHARLES AHN, Yale University — The integration of crystalline oxides and semiconductors has been made possible by the development of techniques that allow crystalline SrTiO3 to be grown on the silicon (001) surface. The most successful approach to realizing these epitaxial oxide-silicon (001) heterostructures requires manipulating substrate temperature and oxygen pressure on a layer-by-layer basis during the deposition of the metal oxide layers. The transition layer between the semiconductor and crystalline oxide is an alkaline earth metal, most often strontium, that is deposited on the silicon surface at around 650 °C. Motivated by the desire to develop a fundamental understanding of this important transition layer, we have studied the surface structures formed by strontium on miscut silicon wafers, which, unlike regular silicon wafers, have a unique surface termination. At high temperatures, this reaction rearranges the top layer of silicon to replace the original top layer with strontium. At low temperatures, this reaction is suppressed, leading to a different, but symmetry related, ordered surface structure. We find that complex oxides can be grown on either surface with comparable crystallinity.

9:12AM V21.00007 ABSTRACT WITHDRAWN

9:24AM V21.00008 Continuum model of surface roughness evolution of a-Si:H films grown by low-temperature PECVD, YEVGEN KRYUKOV, NIK PODRAZA, ROBERT COLLINS, JACQUES AMAR, University of Toledo — Using real-time spectroscopic ellipsometry the evolution of the surface roughness in a-Si:H thin-films grown on smooth c-Si/native oxide substrates by low-temperature plasma-enhanced chemical vapor deposition (PECVD) has been studied as a function of the H2 dilution ratio R = ([H2]/[SiH4]) with 15 ≤ R ≤ 60. The best amorphous Si photovoltaic films correspond to a relatively high dilution ratio (R ~ 60) such that the surface roughness is minimized but close to the amorphous-microcrystalline transition. After a brief period of nucleation of 3D islands, the roughness decreases but then eventually increases rapidly at large bulk layer thicknesses. Using a 3D continuum equation which includes a negative surface tension to take into account the destabilizing effects of short-range attraction and/or shadowing, as well as a smoothing term to take into account surface diffusion we have been able to obtain excellent agreement with experimental results for the evolution of the surface roughness. The dependence of our model parameters on the dilution ratio R is also discussed.
9:36AM V21.00009 In-situ growth of two-terminal silicon nanowires from locally heated cantilevers. CHRISTIAN KALLESOE, DTU Nanotech, Technical University of Denmark, FRANCES ROSS, CHEN-YEN WEN, IBM TJ Watson Research Center, KRISTIAN MOLHAVE, PETER BOGGILD, DTU Nanotech, Technical University of Denmark — Resistively heated crystalline silicon cantilevers extending over the edge of a chip offer excellent control of local growth of nanowires, without heating the entire micro-system. Besides being CMOS compatible, the cantilevers also have a rapid temperature cycling, and furthermore the freestanding cantilevers are suitable for in-situ studies of nanowire growth inside a TEM, offering the possibility of applying electrical fields to direct the growth and growing bridging wires between cantilevers thereby making two-terminal in-situ electrical measurements of nanowires possible. We have used such cantilever loops to study the growth of nanowires in-situ in UHV TEM. Epitaxial growth was observed from the crystalline cantilevers and the rapid temperature cycling ensured a very fast reaction time when crystalizing or melting the catalytic particle. The silicon wires were grown towards a cold cantilever loop, thereby forming bridging nanowires and the nanowire contact was seen to depend on the wetting ability of the gold catalytic particle to the cold cantilever. Furthermore various two-terminal measurements were performed on the bridging silicon nanowires in-situ in UHV.

9:48AM V21.00010 Time-Evolution of the Grain Size Distribution in Random Nucleation and Growth Crystallization Processes. ANDREAS BILL, ANTHONY V. TERAN, Department of Physics & Astronomy, California State University Long Beach, RALF B. BERGMANN, Bremen Institute for Applied Beam Technology (BIAS), 28359 Bremen, Germany — The micromorphology of solids impacts in an essential way their mechanical, electronic, optical or magnetic properties. Hence, it is an important task to characterize properly the granularity of materials. One central quantity providing such information is the grain size distribution. We propose an analytical derivation of this distribution during the random nucleation and growth crystallization process of a $d$-dimensional solid ($d = 1, 2, 3$). We describe how the grain size distribution evolves from early stages of crystallization to its final form when complete crystallization is achieved. We also discuss the remarkable result that for certain classes of nucleation and growth rates the asymptotic limit of large times is a lognormal type distribution. Finally, we apply the theory to the time-evolution of the grain size distribution during solid-phase crystallization of Si-films.

This work is supported by the Research Corporation and by SCAC at CSU Long Beach.

10:00AM V21.00011 ABSTRACT WITHDRAWN

10:12AM V21.00012 Nanocrystalline Silicon Films by HWCVD Method. PURABI GOGOI, HIMANSHU S. JHA, PRATIMA AGARWAL, Department of Physics, IIT Guwahati, Guwahati 781039, India — High quality nano-crystallites embedded amorphous silicon films are deposited using HWCVD technique by varying the substrate temperature $T_S$ (100-350 $^\circ$C) and chamber pressure P (0.08-8mbar). The precursor gas used is semiconductor grade hydrogen diluted silane (10 % silane in hydrogen) from Matheson Inc. Film temperature ($T_F$) is kept constant at 1800 $^\circ$C. The films are characterized by different tools viz. XRD, SEM, TEM, UV-Vis NIR spectroscopy, FTIR and PL. Both XRD and HRTEM studies indicate the presence of Nanocrystallite (size 5-10nm) in these films. The deposition rate ranges from 5-13 Å/Sec, whereas the hydrogen content varies between 2.5-5. The films deposited at high pressure have high deposition rate, low hydrogen content and high band gap. The films are found to be of superior electronic properties suitable for photovoltaic device applications. The tunable band gap, high deposition rate and low hydrogen content is ideal for cost effective device fabrication.

1Work supported by DST, New Delhi.

10:24AM V21.00013 Growth and physical properties of epitaxial GdN and SmN. BEN RUCK, BART LUDBROOK, JOE TRODAHL, ANDREW PRESTON, CLAIRE MEYER, Victoria University, Wellington, IAN FARRELL, STEVE DURBIN, ROGER REEVES, University of Canterbury, Christchurch, MATTHIAS KUBEL, Victoria University, Wellington, LAURENT RANNO, Institute Neel, Grenoble — The epitaxial growth and passivation of GdN and SmN by pulsed laser deposition on [100] YSZ substrates has been refined. We report on the growth kinetics, including the relaxation of the films, and the incorporation of oxygen at the substrate-film interface. Magnetic susceptibility measurements confirm a Tc of 70K and small coercive field for GdN. Resistivity measurements show an anomalous peak at Tc, while magnetic transport measurements indicate the films are electron doped to degeneracy, and show a strong anomalous Hall contribution below Tc.

10:36AM V21.00014 Synthesis and Magnetism of High Curie Temperature Prussian Blue Analogue Molecular Nanomagnet-Chromium Cyanide Molecule Nanowire Arrays. PINGHENG ZHOU, 1 Center for Advanced Microstructures and Devices (CAMD), Louisiana State University, Baton Rouge, LA 70806, DESHENG XUE, JINLI YAO, Key Laboratory for Magnetism and Magnetic Materials of MOE, Lanzhou University, Lanzhou 730000, China — The goal to synthesize molecular nanomagnets that exhibit spontaneous magnetic ordering close to room temperature might enable one to apply them in the fields of magnetic memory devices and microelectronics. Chromium cyanide molecule nanowires arrays with diameters of about 50 nm and lengths up to 4μm have been synthesized by an electrodeposition technology based on anodizing anodic aluminum oxide films. Characterization measurements show that the oxidation state of the chromium ions in the chromium cyanide nanowires can be expressed as Cr$_{3+}$-CN-Cr$_{3+}$.$\cdot$ Magnetic properties measurements indicate that the Curie temperature of chromium cyanide nanowire is 200 K, which is closer room temperature compared with current molecular nanomagnet systems.

10:48AM V21.00015 ABSTRACT WITHDRAWN

Thursday, March 19, 2009 8:00AM - 10:48AM

Session V22 GMAG DMP FIAP: Focus Session: Dilute Magnetic Oxide Semiconductors 324

8:00AM V22.00001 A few ways in which LDA et al can produce a wrong description of magnetism in oxides. ALEX ZINGER, S. LANY, H. RAEBIGER, NREL — Part of the anarchy that exist in the literature regarding conflicting predictions of ferromagnetism in oxides can be attributed to problems in LDA and its application:(1) LDA et al tend to place the oxide conduction band minima CBM) at much too deep energies; transition-metal impurity levels then incorrectly appear within the (delocalized) LDA continuum (instead of in the gap). This leads to overly optimistic result of long-range magnetism. This is not fixable via LDA+U.(2) Oxides are naturally off-stoichiometric, exhibiting significant concentration of indigenous free-carriers that greatly affect the occupancy of impurity levels. Yet, such non-stoichiometry is ignored in many calculations using instead a perfect host crystals. This alters the magnetic properties. (3) LDA Predicted magnetism in defected oxides without TM impurities often rely on the defect orbitals (e.g, cation vacancy) being equally delocalized over all of its ligand atoms. While inherent to LDA, experiment, as well as more correlated approaches reveal that such orbitals are "locked" instead onto a single ligand. This symmetry-breaking causes them to become too localized for (percolative) magnetism. We show here how such problems might be fixed.

1 Funded by DOE-SC-BES-DMSE under NREL Contract DE-AC36-08GO28308.
8:12AM V22.00002 First-principles study of the effect of vacancies on magnetic properties. YOSHI KAWAZOE, Tohoku University, QIANG SUN, Peking University and Virginia Commonwealth University, PURU JENA, Virginia Commonwealth University — Due to the high solubility of Co in ZnO, the magnetic properties of Co-doped ZnO thin films have been extensively studied experimentally. Unfortunately, these results have led to diverse conclusions. To better understand the origin of the controversial experimental findings, we have carried out detailed theoretical studies, focusing on the role of concentration and distribution of Zn and O vacancies on the magnetism of Zn1-xCoxO thin films. We find that when Co atoms are substitutionally doped in ZnO thin films without any defects, the magnetic coupling between Co atoms is intrinsically anti-ferromagnetic. The coupling, however, changes to ferromagnetic when sufficient oxygen vacancies are introduced. On the other hand, Zn vacancies stabilize the anti-ferromagnetic coupling, in sharp contrast with that found in Zn1-xMnxO thin films. Our theoretical studies explain the origin of the different magnetic behavior observed experimentally.

8:24AM V22.00003 On the possibility of ferromagnetism in MgX (X = O, S, Se) with/without conventional magnetic atoms. VAN AN DINH, ISIR, Osaka University, KAZUNORI SATO, HIROSHI KATAYAMA-YOSHIDA — We present a first principle study on the half-metallicity and ferromagnetism in rock salt MgZ (Z = O, S and Se) with and without conventional magnetic elements. The electronic structure, effective exchange coupling constant and chemical pair interaction are calculated within SIC-LSDA. The Curie temperature is predicted by performing Monte Carlo simulation. A possibility of spinodal decomposition is investigated and simulated. For transition-metal-doped MgO, our results reflect the observation in the experiment [1]. Without oxygen vacancy, Co- and Ni-doped MgO is anti-ferromagnetic. Except Ti and Cr, another transition metals cause the anti-ferromagnetic behavior in MgO. The ferromagnetism can be stabilized by oxygen vacancies. Oxygen vacancies also change the chemical interaction trend of transition metal atoms, and cause an inhomogeneous distribution in MgO. It is also found that N atoms which substitute for anions can introduce the half-metallic ground state and ferromagnetism in MgZ. Monte Carlo simulation shows the above room temperature ferromagnetism in MgO NO Z. Nitrogen atoms in MgO and MgS have a tendency to create clusters, whereas the distribution of N atoms in MgSe is homogeneous at dilute regime. [1]. J. Narayan et al., Appl. Phys. Lett. 93 (2008) 082507.

8:36AM V22.00004 Ferromagnetism in MgO by Nitrogen Doping. CHEHAN YANG, MAHESH SAMANT, STUART PARKIN, IBM Almaden Research Center — The new group, dilute ferromagnetic oxide and nitride, provides a promising technology potential to combine the magnetic (TM) and electronic properties. Studies in creating ferromagnetism in thin films of doped oxide materials without the inclusion of transition metal (TM) or rare-earth (RE) metal have been speculated in recent years. However, there have been many reports of ferromagnetism in large numbers of different material systems with poor control and reproducibility of these data. Our interest is exploring the possibility of ferromagnetism in oxide and nitride films without the introduction of any TM or RE elements. In this study, we have successfully incorporated substantial amounts of nitrogen up to 13 at% into MgO films using molecular beam epitaxy (MBE) technique. N-doped MgO films were carried out by evaporating the Mg in the presence of both atomic oxygen and nitrogen from two different RF sources. Upon the post-annealing, N atoms generate holes on oxygen and so create magnetic moment as high as 0.4 µB per N. In undoped MgO films, no magnetic signature was seen either in the as-deposited film or the film after annealing, which is a strong indication that the moment arises from the N dopants. The pre-edge feature of oxygen K-edge measured in Near Edge X-ray Absorption Fine Structure (NEXAFS) shows apparent evidence for the substitution of nitrogen for oxygen after post-annealing.

8:48AM V22.00005 Electric field control of magnetic semiconductor (Zn,Co)O. HYEON-JUN LEE, ERIK HELGREN, FRANCES HELLMAN, Dept. of Physics, Univ. of California, Berkeley — The magnetic transport of a conducting Al(2%) doped (Zn,Co)O field-effect transistor is investigated at low temperature (2-10 K). The Al doped (Zn,Co)O channel layer (~26 nm-thick) was deposited by magnetron sputtering at 550°C and processed into a 40 µm thick Hall bar geometry by photolithography and wet etching. An 80nm-thick AlOx layer was deposited at room temperature as the insulating barrier and Cr/Au was used as electrodes. The Hall effect and sheet resistance were measured from 2 - 10 K as a function of temperature, magnetic field and gate electric field. For gate electric field E=0 V/cm, the electron concentration is 2.58 x 10¹⁴/cm² at 5 K and there is no saturation of magnetic moment with increasing gate electric field at low temperature. This research was supported by both DOE and WIN.

9:00AM V22.00006 Electron mediated ferromagnetism in cobalt doped ZnO. SU-HUAI WEI, ARON WALSH, JUAREZ L.F. DA SILVA, National Renewable Energy Laboratory — The potential to simultaneously tune both charge and spin in spintronic materials has lead to great interest in searching room temperature dilute ferromagnetic semiconductors. Among them, cobalt doped ZnO has become a focus of attention in creating ferromagnetism in thin films of doped oxide materials without the inclusion of transition metal (TM) or rare-earth (RE) metal have been speculated in recent years. However, there have been many reports of ferromagnetism in large numbers of different material systems with poor control and reproducibility of these data. Our interest is exploring the possibility of ferromagnetism in oxide and nitride films without the introduction of any TM or RE elements. In this study, we have successfully incorporated substantial amounts of nitrogen up to 13 at% into MgO films using molecular beam epitaxy (MBE) technique. N-doped MgO films were carried out by evaporating the Mg in the presence of both atomic oxygen and nitrogen from two different RF sources. Upon the post-annealing, N atoms generate holes on oxygen and so create magnetic moment as high as 0.4 µB per N. In undoped MgO films, no magnetic signature was seen either in the as-deposited film or the film after annealing, which is a strong indication that the moment arises from the N dopants. The pre-edge feature of oxygen K-edge measured in Near Edge X-ray Absorption Fine Structure (NEXAFS) shows apparent evidence for the substitution of nitrogen for oxygen after post-annealing.

9:12AM V22.00007 Origin of the co-dopant induced enhancement of ferromagnetism in (Zn,Mn)O. YAN ZHU, JUEXIAN CAO, Department of Physics and Astronomy, University of California, Irvine, California, Z.Q. YANG, Surface Physics Laboratory (National Key Laboratory), Fudan University, Shanghai 200433, China, RUQIANG WU, Department of Physics and Astronomy, University of California, Irvine, California 92617-4575, USA — Using the density functional calculations, we elucidate the mechanism of co-dopant induced enhancement of ferromagnetism of (Zn,Mn)O. Li and Cu atoms tends to segregate toward Mn atoms and strongly promote the ferromagnetic coupling via either RRKKY or superexchange interaction. The hole states produced by either Li or Cu are rather delocalized and they are efficient in mediating magnetic ordering. These findings shed new light for the design of dilute magnetic semiconductors with co-dopants for spintronic applications.

9:24AM V22.00008 Synthesis and Magnetic Properties of Cobalt doped ZnO Nanowires. RA-MAKRISHNA PODILA, JIAN HE, AMAR NATH, APPARAO RAO, DEPARTMENT OF PHYSICS AND ASTRONOMY, CLEMSON UNIVERSITY, CLEMSON, SC, 29634 COLLABORATION, DEPARTMENT OF CHEMISTRY, THE UNIVERSITY OF NORTH CAROLINA AT ASHEVILLE, ASHEVILLE, NC, 28804 COLLABORATION — Here we report the synthesis of cobalt (Co) doped ZnO nanowires using a chemical vapor deposition technique. About 50 mM aqueous solution of ZnCl₂ and Co (CH₃COO)₂ was injected (rate of 0.1ml/min)into a quartz tube reactor maintained at 550 °C. A constant flow (10:1) of O₂ and H₂ was maintained at 500 sccm. The as-prepared nanowires are typically ~1-2 micrometers in length and tens of nanometers in diameter. X-ray diffraction, scanning electron microscopy and energy dispersive X-ray spectroscopy were employed to confirm the presence of the Co atoms in the nanowires. Significant magnetic signature was observed in the 2 atomic % Co-doped ZnO nanowires with a coercive field of 50 Oe. Furthermore, no saturation of magnetic moment was observed up to a field of 5T and 5K. A Curie-Weiss law fit to the temperature dependent magnetic susceptibility data yielded a magnetic moment µ = 1.99µB for Co²⁺ ion, consistent with the low spin state. Based on Hall measurements and Seebeck coefficient data, the nature of the carriers and origin of magnetism in Co doped ZnO nanowires will be presented.
observed. The magneto-resistive properties are analyzed with respect to recent models of spin-dependent scattering in magnetic semiconductors.

In materials science, the properties of magnetic semiconductor (MSS) and metallic nanostructures, such as nanowires and nanoparticles, have been extensively studied due to their potential applications in spintronics and other magnetic devices. For example, magnetic semiconductor (MSS) and metallic nanostructures, such as nanowires and nanoparticles, have been extensively studied due to their potential applications in spintronics and other magnetic devices. For example, magnetic semiconductor (MSS) and metallic nanostructures, such as nanowires and nanoparticles, have been extensively studied due to their potential applications in spintronics and other magnetic devices. For example, magnetic semiconductor (MSS) and metallic nanostructures, such as nanowires and nanoparticles, have been extensively studied due to their potential applications in spintronics and other magnetic devices.

References...

1. DST, India

9:48AM V22.00010 Magnetism of TiO and TiO2 Clusters, XIAOHUI WEI, RALPH SKOMSKI, B. BALAMURUGAN, Z. SUN, University of Nebraska, D.J. SELLMYER, UNIVERSITY OF NEBRASKA TEAM — Ferromagnetism in wide-bandgap semiconductors has sparked interest due to its potential applications in spintronic devices. Previous research has focused on dopant TiO2 thin films, with little work on undoped TiO2 and no report on TiO clusters. To investigate the magnetism of small TiO clusters, TiO2 and TiO clusters with sizes from 15 to 50 nm were grown by gas condensation and examined with TEM, AFM, XRD, and SQUID. Ferromagnetism was found within the investigated temperature range of 10 to 400 K for all clusters including TiO. Interestingly, all clusters exhibit a magnetization enhancement after exposure in air for an extended time, which is probably due to the generation of oxygen vacancies and of Ti3+ or Ti4+, whose coupled spins may create the observed ferromagnetism. The relationship between cluster structure, size, defects and magnetism will be discussed. - This research is supported by NSF-MRSEC, ONR and NCMN. 1 J. M. D. Coey, Curr. Opin. Solid State Mater. Sci. 10, 83 (2006) 2 S. Yoon, J. Phys.: Condens. Matter 18, L355 (2006)
8:00AM V23.00001 Phase separation in hydrogen-helium mixtures at high pressure, MIGUEL MORALES, University of Illinois at Urbana-Champaign, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, DAVID CEPERLEY, University of Illinois at Urbana-Champaign, CARLO PIERLEONI, University of L’Aquila, L’Aquila (Italy), SEBASTIAN HAMEL, KYLE CASPERSSEN, Lawrence Livermore National Laboratory — We study the properties of hydrogen-helium mixtures at Mbar pressures and intermediate temperatures (4000 to 10000 K) using first-principles molecular dynamics simulations. Our main goal is to calculate the temperature, as a function of pressure, at which helium becomes insoluble in dense metallic hydrogen. We perform an extensive study of the equation of state of the mixture as a function of density, temperature, and composition and, together with a variety of thermodynamic integration techniques, we calculate the Gibbs free energy of mixing. We will show how to calculate the entropic contribution of the free energy using coupling constant integration methods, which allows us to directly calculate immiscibility temperatures without the need to resort to approximations of the entropy of mixing. These results are relevant to models of the interior structure and evolution of Jovian planets. We find demixing temperatures that are sufficiently high to cross the planetary adiabat of Saturn at pressures around 5 Mbar, implying the existence of partially miscible regions over a significant portion of the interior of the planet.

8:12AM V23.00002 Molecular dynamics simulations of electron-ion temperature equilibration in an SF6 plasma, LORIN X. BENEDICT, JAMES N. GLOSFI, DAVID F. RICHARDS, FREDERICK H. STREITZ, STEFAN P. HAU-RIEGE, FRANK R. GRAZIANI, Lawrence Livermore National Lab, MICHAEL S. MURLILLO, JOHN F. BENAGE, Los Alamos National Lab — We use classical MD to investigate electron-ion temperature equilibration in a two-temperature SF6, plasma. We choose a density of 1.0\times10^{25} (dissociated) SF6 molecules per cm^3 and initial temperatures of T_e \sim 100 \text{ eV} and T_i \sim 15 \text{ eV} in accordance with experiments currently underway at Los Alamos National Laboratory. Our computed relaxation time is significantly longer than that predicted by the classic theory of Landau and Spitzer. Similar discrepancies are found when comparing to predictions made be more recent theories of electron-ion equilibration. These differences should be large enough to be measured in the upcoming experiments.

8:24AM V23.00003 Optical signature of the OCP crystallization in a boron plasma, FLAVIEN LAMBERT, STÉPHANE MAZEVET, JEAN CLÉROUIN, CEA, DAM, DIF — We have calculated the DC conductivity of a boron plasma along the 1 eV isotherm up to 25 times the normal density. We use the free and orbital free molecular dynamics coupled with, respectively, the Kubo-Greenwood formulation and the semi-classical Ziman theory. We find that the DC conductivity obtained using a full quantum mechanical treatment exhibits a significant jump at the one component plasma phase transition — specifically the OCP crystallization — jump that is not reproduced using the semi-classical Ziman description. This difference — reaching up to a factor of four — remains well beyond the phase transition and up to the highest density explored. This shows that a full quantum mechanical treatment of the optical and electrical quantities is required in this regime even if semi-classical theories are reliable to obtain both the thermodynamical, and, ionic dynamical and structural properties.

8:36AM V23.00004 Mixtures in the Warm, Dense Matter Regime, LEE A. COLLINS, Los Alamos National Laboratory — The bulk of normal matter from planets to the intergalactic medium exists as a composite of various elemental constituents. The interactions among these different species determine the basic properties of such diverse environments. For dilute systems, simple gas laws serve well to describe the mixing. However, once the density and temperature increase, more sophisticated treatments of the electronic component and dynamics become necessary. For the warm, dense matter (WDM) region \[10^{22} - 10^{25} \text{ atoms/cm}^3 and 300K - 10^6 \text{ K}, quantum Monte Carlo and molecular dynamics, utilizing finite-temperature density functional theory (DFT), have served as the basic exploratory tools and benchmarks for other methods. The computational intensity of both methods, especially for mixtures, which require large sample sizes to attain statistical accuracy, has focused considerable attention on mixing prescriptions based on the properties of the pure atomic constituents. Though extensively utilized in many disciplines, these rules have received very little verification[1,2]. We examine the validity of such rules as density and pressure mixing, for several systems and concentrations by comparing against quantum calculations of the fully-interacting composite. We find considerable differences in some regimes, especially for optical properties. We also probe dynamical properties such as diffusion and viscosity as well as the role of impurities. Finally, as a means of extending DFT results to higher temperature regimes, we also study orbital-free molecular dynamics (OFMD) approaches[3] based on various approximations to the basic density functional. These OFMD schemes permit a smooth transition from the WDM region to simpler one-component plasma and ideal gas models. Research in collaboration with J.D. Kress (LANL), D.A. Horner (LANL), and Flavien Lambert (CEA).


1Work performed under the auspices of the U.S. Department of Energy.

9:12AM V23.00005 Electrical Conductivity of Synthetic Uranus, SEBASTIEN HAMEL, ERIC SCHWEGLER, LLNL — Mixtures of accreted water, ammonia, and methane at high pressures and temperatures are thought to be major components of the giant planets such as Uranus and Neptune. The pressures and temperatures in their deep interiors can reach several Mbar and several thousands Kelvin, conditions corresponding to the fluid phase. At such extreme interior conditions it is expected that these molecules react chemically to produce a complex mixture. Observables properties such as the magnetic field of these planets are thought to be determined by the physical and chemical properties of matter within this water mixture layer. Using quantum molecular dynamics, we explore the properties of water mixtures at planetary conditions. In particular we discuss the electrical conductivity at high pressure and high temperature of those mixtures in comparison to pure water. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

9:24AM V23.00006 Magnetism and vibrations in the phase ϵ of Oxygen, TUAN ANH PHAM, University of California, Davis, RALPH GEBAUER, SANDRO SCANDOLO, The Abdus Salam International Centre for Theoretical Physics — Sandwiched between a set of magnetic phases at lower pressure, and a non magnetic phase at higher pressure, the magnetic state of phase ϵ of oxygen has so far been elusive, together with its crystal structure. Neutron diffraction data indicate absence of antiferromagnetism, but do not exclude a ferromagnetic order. The recent refinement of the internal atomic positions from single-crystal diffraction finally provides us with a correct structural model to study the possible occurrence of a magnetic ground state. By employing non-collinear spin-polarized density-functional theory we show that the ground state of ϵ-O2 is non magnetic. We also calculate vibrational spectra and show that ϵ-O2 possesses an additional vibron mode with large Raman cross section, not seen in experiments yet.

9:36AM V23.00007 Ab-initio calculations of the X-ray absorption spectra of shocked compressed aluminum, STEPHANE MAZEVET, VANINA RECOULES, GILLES ZERAH, CEA-DIF F91297 Arpajon France — Molecular dynamics (MD) simulations, using density functional (DF) electronic structure techniques, provide a powerful, predictive tool for examining materials from solids to plasmas over a wide range of densities and temperatures. Using the Kubo-Greenwood formulation, we can access to the frequency-dependent electrical conductivity as well as additional optical properties consistent with the Equation of State. Due to the use of pseudopotentials, the calculations of these properties have, so far, been limited to low photon frequencies, i.e. below 100eV, where only the valence electrons contribute. We recently extended those calculations into the X-ray domain within the PAW formalism. This allows us to describe for the first time, X-ray absorption spectra of shocked compressed aluminum from an ab-initio standpoint.
9:48AM V23.00008 High-pressure spectroscopic studies on solid germane$^1$, XIAOJIA CHEN, VIKTOR V. STRUZHKIN, ZHEN-XIAN LIU, MÜHETAER AIHAI, YUE MENG, HOU-KWANG MAO, RUSSELL J. HÉMELY, Carnegie Institution of Washington, Washington, DC 2005, CHAO ZHANG, RUI-QIN ZHANG, City University of Hong Kong, Kowloon, Hong Kong, YANLING LI, HAI-QING LIN, The Chinese University of Hong Kong, Shatin, Hong Kong — We performed extensive spectroscopic studies on dense germane up to 110 GPa. Pressure — temperature phase diagram has been established from Raman and infrared spectra. There is no any trace of decomposition of Ge and H$_2$ over the pressure range studied. Infrared measurements provide spectroscopic evidence of the metallization of this material at pressure around 16 GPa which is much lower than that observed in sister system - silane. Angle-dispersive powder x-ray diffraction studies reveal that only a structural transition is accompanying when germane enters its metallic state. These experimental observations are examined by ab initio calculations. The theoretical results of the electronic, lattice dynamical, and superconducting properties of metallic phase of this material are also presented.

$^1$This work was supported by the DOE, NSF, HKGRC, and NSFC.

10:00AM V23.00009 High pressure optical properties of sodium, AMY LAZICKI, ALEXANDER GONCHAROV, VIKTOR STRUZHKIN, ZHENXIAN LIU, Carnegie Institution of Washington, EUGENE GREGORYANZ, CHRISTOPHE GUILLAUME, University of Edinburgh, HO-KWANG MAO, RUSSEL HEMLEY, Carnegie Institution of Washington — Sodium displays significant complexity at high pressure. The melting temperature increases with pressure in its dynamically stable range. The FS filling constant and FS topology transitions under pressure mostly account for the different superconductivity between the molecular and atomic phases.

$^1$This work was supported by 973 Program of China (2005CB724400)

10:12AM V23.00010 Influence of Fermi Surface Topology on Superconductivity in High-Pressure Phases of Silane$^1$, TIAN CUI, XILIAN JIN, State Key Lab of Superhard Materials, Jilin University — Both a semimetallic molecular phase with P$\bar{2}1$/m symmetry and a metallic atomic phase with P$\bar{2}$1/c symmetry are found using ab initio geometry optimization method from initial configurations of random molecular SiH$\text{3}$ and atoms Si and H, respectively. The molecular phase shows a pressure-induced metallization, which can be described quantitatively by Fermi surface (FS) filling constant defined in our work. The lower superconducting critical temperature (Tc) about 16.2 K at 175 GPa and its peculiar superconductivity behavior that its Tc decreases initially and increases later with pressure agree with a recent experimental results. Different electron-phonon coupling mechanisms are uncovered during the increase and decrease of Tc with pressure. The atomic phase shows a higher Tc of about 47 K at 190 GPa and its Tc increases with pressure in its dynamically stable range. The FS filling constant and FS topology transitions under pressure mostly account for the different superconductivity between the molecular and atomic phases.

$^1$This work was supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

10:24AM V23.00011 Structural Properties of Superconducting CaLi$\text{2}$ At High Pressures, HAHN-BIDT RHEE, WARREN PICKETT, RICHARD SCALETAR, UC Davis Physics Dept, WILLIAM EVANS, LLNL High Pressure Physics Group, DAVID YOUNG, Louisiana State Univ Dept of Physics & Astronomy — The hexagonal Laves phase of CaLi$\text{2}$, a superconductor at high pressures, has been studied in the diamond anvil cell at varying pressures and temperatures. CaLi$\text{2}$ is known to have a maximum superconducting transition temperature of 13 K at 40 GPa. X-ray diffraction measurements were done up to 40 GPa, from room temperature down to 10 K, and phase stability in relation to pressure and temperature has been examined. We present our study to provide more insight into phonon-mediated superconductors and simple-metal systems such as Li. This work was performed under the auspices of the US DOE by LLNL under Contract DE-AC52-07NA27344 and under Contract DE-FG01-06NA26204. HPCAT use is supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

10:36AM V23.00012 Fe K pre-edge of Fe$_\text{2}$O$_\text{3}$ at High Pressure$^1$, SHIBING WANG, Department of Applied Physics, Stanford University, WENDY MAO, Department of GE, Stanford University, Photon Science, SLAC National Accelerator Laboratory, YONG CAI, Brookhaven National Laboratory, NOZOMU HIRAOKA, HIROFUMI ISHII, National Synchrotron Radiation Research Center, Taiwan, YANG DING, YUMING XIAO, PAUL CHOW, HO-KWANG MAO, JINFU SHU, Geophysical Laboratory, Carnegie Institution of Washington, CHICHANG KAO, Brookhaven National Laboratory — Hematite (α-Fe$_\text{2}$O$_\text{3}$), an archetypal 3d transition metal oxide and important earth mineral, undergoes a series of electronic transitions and structural changes at high pressure. At ambient conditions, Fe$_\text{2}$O$_\text{3}$ adopts the α-Al$_\text{2}$O$_\text{3}$ structure and is an antiferromagnetic Mott insulator, with five 3d electrons on a high-spin state. Upon increasing pressure, it transforms from a high-spin state to a low-spin state in the 40-70 GPa range. Here we report experimental results for the Fe K-edge spectra of Fe$_\text{2}$O$_\text{3}$ collected in-situ at high pressure using synchrotron x-ray absorption spectroscopy in partial fluorescence yield geometry. The pre-edge features give explicit information about the crystal field splitting energy (CFSE) of octahedrally coordinated Fe$^{\text{3+}}$ in Fe$_\text{2}$O$_\text{3}$ as a function of pressure, mapping the electronic structure (high-spin to low-spin) transition. The K-α emission spectra at high pressure are also presented.

$^1$S. Wang and W. Mao are supported by NSF and DOE-NNSA(CDAC).

10:48AM V23.00013 High Pressure Phase Transitions in FeO from Density Functional Theory, Quantum Monte Carlo and Dynamical Mean Field Theory, LUKE SHULENBURGER, KEN ESLER, Geophysical Laboratory, Carnegie Institution, SERGEJ SAVRAŠOV, Department of Physics, University of California, Davis, JONGNIM KIM, University of Illinois at Urbana-Champaign, R. E. COHEN, Geophysical Laboratory, Carnegie Institution — FeO has a rich behavior under pressure, exhibiting a structural phase transition as well as an insulator-metal transition and a spin collapse. The electronic transitions have been particularly difficult to explain because of the failure of Density Functional Theory (DFT) to capture the electronic state of FeO. We present results from three different methods to better understand the nature of this material. First, from DFT calculations we explore competing explanations for the spin collapse, finding that the increase in bandwidth is at least as important as the crystal field splitting. Additionally, we find that the ligand field effects are responsible for the majority of the change in the local energy levels on the Fe rather than the electrostatic crystal field effect. Secondly, we have performed Dynamical Mean Field Theory (DMFT) calculations. From these we find that the metal insulator transition involves the reorganization of the existing bands and not the appearance of new states at the Fermi level. Finally we test the validity of the approximate results obtained by DFT and DMFT by performing highly accurate Diffusion Monte Carlo calculations.
8:00AM V24.00001 Broken Optical Symmetry in DNA-SWNT Hybrids: Spectroscopic Signaling of the Helical Wrap* SLAVA V. ROTKIN, Lehigh University — Functionalizing single-stranded DNA on a single-wall carbon nanotube (SWNT) has allowed isolating individual tubes, making them soluble, and separating SWNTs according to their chirality. Such strong technological impact motivated our study of the optical properties of the DNA-SWNT hybrids, commonly used now for the solution-based fabrication and experiments. The helicity of the DNA wrap may interfere with the intrinsic Hamiltonian of the SWNT and result in bandstructure modulation. Our modeling predicts a symmetry lowering in the hybrid due to the Coulomb potential of the regular helical wrap of the ionized backbone of the ssDNA, followed by the qualitative changes in the cross- or circularly polarized SWNT absorption spectrum (with or little change in the parallel polarization). In particular, we predict the appearance of a new peak in the cross-polarized absorption of the ssDNA-SWNT at a frequency lower than that of all allowed transitions in the bare tube. Such effect can be used for optical identification of the wrap at sufficient ssDNA coverage. Wrap signaling happens also via another optical effect, a strong circular dichroism even in the complex with an achiral SWNT, and even at the frequencies where ss-DNA has no absorption features at all. Symmetry of the wrap is central to determine such a circualar dichroism of the hybrid. Having in mind that the exact geometry of a DNA wrap for an arbitrary tube is not precisely known yet, we put forward a general model capable of tracking optical effects, varying the parameters of the wrap and/or tube diameter. For various ssDNA backbone helical angles and for various tubes we predict different absorption spectra, though a general qualitative feature of the helical symmetry breaking, the appearance of new Van Hove singularities and circular dichroism, must be present.

1NSF CMS-0609050, DoD-ARL W911NF-07-2-0064, ACS PRF 46870-G10

8:36AM V24.00002 Color Detection Using Chromophore-Nanotube Hybrid Devices , XINJIAN ZHOU, THOMAS ZIFER, BRYAN WONG, KAREN KRAFCIK, FRANÇOIS LÉONARD , ANDREW VANCE. Sandia National Laboratories — In this talk, we will present a nanoscale color detector based on a single-walled carbon nanotube functionalized with azobenzene chromophores, where the chromophores serve as photoabsorbers and the nanotube as the electronic read-out. By synthesizing chromophores with specific absorption windows in the visible spectrum and anchoring them to the nanotube surface, we demonstrate the controlled detection of visible light of low intensity in narrow ranges of wavelengths. Our measurements are consistent with those proposed from first-principles density functional theory showing that a single nanotube can serve as a molecular optical detector, similar to several known macroscopic devices. We show that by investigating the optical properties of these hybrid systems using density functional theory. Including the contributions for the non-local dispersive interactions, we examine the unique mechanical and electronic properties of nanotubes with the desired optical properties of π conjugated chromophores. We investigate structural, cohesive and optical properties of various fullerene derivatives using density functional theory. Including the contributions for the non-local dispersive interactions, we examine in a systematic manner the effect of tube diameter and chirality on the stability and bonding characteristics of the peapod as well as the position of the molecule in the dielectric and loss functions due to transitions between the states of the molecule and the nanotube.

8:48AM V24.00003 Spectral Features of Carbon Nanotube Films Changeable With Increasing Thickness , JOHN H. LEHMAN, The National Institute of Standards and Technology, KATALIN KAMARAS, ARON PEKKER, Hungarian Academy of Sciences, KATHERINE E. HURST, The National Institute of Standards and Technology, D.B. TANNER, University of Florida — We have investigated an apparent contradiction with respect to optical spectroscopy of carbon nanotube films. The measured absorbance shows “inverted” features: local maxima for dilute suspensions correspond to local minima for thick films. The inversion is reconciled by taking into account the saturation of absorption in thick films, when all the light is absorbed in the sample. In this case, the measured direct absorption is (1-R), and independent of thickness. Kramers-Kronig analysis of transmittance data, which provides a means to model absorbance for material ranging from nearly transparent to almost completely opaque, provides values of refractive index for a film of nanotubes. (Borondics et al., PRB 74, 045431 (2006)). From these values, we determined (1–R~T) at many values of the film thickness. This calculation is corroborated with measurements based on the spectral responsivity of a pyroelectric detector and the absolute absorbance of the films. These results are consistent with data on nanotube suspensions by Zhang et. al. (J. Phys. Chem B, 108, 8136 (2004)), representing the limiting case of transparent samples, as well as films by Lehman et. al. (J. Phys. Chem. C, 112, 11776–11778 (2008)) representing the other limiting case of completely opaque samples.

9:00AM V24.00004 Light emitting peapods: A first-principles study , MATUS MILKO, TAYEBEH MOVALI-ROOY, CLAUDIA AMBROSCH-DRAML, Chair of Atomic Modelling and Design of Materials, University of Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — Nanohybrids i.e. single wall carbon nanotubes with encapsulated organic molecules have been proposed for opto-electronic devices as they combine the unique mechanical and electronic properties of nanotubes with the desired optical properties of π-conjugated molecules. We investigate structural, cohesive and optical properties of various fullerene derivatives using density functional theory. Including the contributions for the non-local dispersive interactions, we examine in a systematic manner the effect of tube diameter and chirality on the stability and bonding characteristics of the peapod as well as the position of the molecule inside the tube. We find that these systems are almost exclusively van-der-Waals bound. Based on a series of oligo-thiophenes encapsulated into zig-zag nanotubes, we explore how the presence of the molecules inside the cavity can alter the electronic and optical properties. In particular, we inspect new features in the dielectric and loss functions due to transitions between the states of the molecule and the nanotube.

9:12AM V24.00005 Friction and Stability of Carbon Onions Films in Vacuum R.A. AL-DUHAILEB, Michigan State University, B.W. JACOBS, Sandia National Laboratories, CA, M.A. CRIMP, V.M. AYRES, Michigan State University, A. HIRATA, M. HORIKOSHI, Tokyo Institute of Technology, Japan, M.G.I. GALINATO, N. LEHNERT, University of Michigan — Planar graphite is a state-of-the-art low friction solid lubricant. However, in vacuum environments, graphite-based solid lubricants require potentially harmful heavy metal additives to maintain tribological performance. Recent experiments by our group indicate that carbon onions show excellent tribological performance (~0.03 friction coefficient) without the addition of heavy metal additives. They are therefore good candidates for environmentally benign solid lubricants for use in vacuum. Carbon onion film stability to prevent exposure of un-lubricated surfaces is also an important issue. Tribological performance assessed using ball-on-disk friction measurements equivalent to a 10 m sliding distance indicated that a 15 wt.% solution at 80 °C peroxide oxidation treatment improved the film stability. In the present work, carbon onion friction and film stability are correlated with fundamental structural and chemical properties investigated by high-resolution transmission electron microscopy (HRTEM), electron energy loss spectroscopy (EELS) and multi-wavelength micro-Raman spectroscopy at 77K.

9:24AM V24.00006 Computational Study on the Structural and Electronic Properties of Various Fullerene Derivatives* SORA PARK, JEUNG SUN AHN, Department of Physics, Kyung Hee University, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using ab initio density functional theory, we investigate the structural and electronic properties of various fullerene derivatives. The equilibrium structures of various additives adsorbed on a fullerene molecule forming fullerene adducts are computed through the geometry relaxation. For a given fullerene adduct, we also calculate the optimum configuration with a different number of additives. In tandem with the structural studies, we calculate the dependence of the HOMO-LUMO gap of each fullerene adduct on the number of additives, and on their relative positions and orientations. Further, using the GW approximation, we also examine the quasiparticle electronic structure of various fullerene derivatives.

*This work was supported by the Seoul Research and Business Development Program (Grant No. 10583)
9:36AM V24.00007 Diffusion of Various Molecules through Crystalline C$_{60}$ Solid and their Electronic and Vibrational Properties$^1$, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — First-principles density functional theory is used to study the diffusion of various molecules including diatomic molecules, inert gas molecules, and small metal atoms, and so on, through the C$_{60}$ solid. For each case, the energy surface of a diffusion path is calculated while performing full geometry relaxation of the whole system. Such studies are performed while changing the concentrations of diffusing molecules. The effects of these molecules on the electronic properties of C$_{60}$ solid are also examined. Especially for diatomic molecules, such as H$_2$, N$_2$, and O$_2$, their frequency shifts are calculated relative to their corresponding counterparts.

This research was supported by the Kyung Hee University Research Fund in 2008 (KHU-20081558).

9:48AM V24.00008 Simulation of Fe$_n$-doped C$_{60}$ Monolayer on h-BN/Ni (111)$^1$, LAN LI, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — We have performed first-principles calculations based on density functional theory to investigate the structural, electronic structure and magnetic properties of Fe$_n$-C$_{60}$ complexes. Interfaces that consist of a C$_{60}$ monolayer, a supporting h-BN/Ni (111) layers, and the transition metal Fe$_n$ (n = 1-4 & 15) have been thoroughly characterized. Electron transfer has been observed from the Fe ions to the C$_{60}$ molecules, which leads to the domination of ionic character on the Fe-C$_{60}$ bonding. Furthermore, the Fe$_n$-doped C$_{60}$ systems show strong hybridizations between s-, d- orbitals of Fe atoms and p-orbital (γ-like) of C atoms. The spin of the net transferred electrons from Fe$_n$ to C$_{60}$ is spin minority, which leads to a magnetic moment in C$_{60}$ opposite to the total magnetic moment of the system. All of the electronic structure calculations have been performed in generalized gradient approximation (GGA) and local density approximation (LDA). In Fe$_n$C$_{60}$ and Fe$_{15}$C$_{60}$ systems, we have also performed GGA+U and LDA+U calculations for comparison.

This work is supported by the U.S. Department of Energy.

10:00AM V24.00009 Superatom states in an endohedral fullerene$^1$, TIAN HUANG, MIN FENG, JIN ZHAO, HRVOJE PETEK, Dept. of Physics and Astronomy, University of Pittsburgh, SHANGFENG YANG, LOTHAR DUNSCH, Group of Electrochemistry and Conducting Polymers, Leibniz-Institute for Solid State and Materials Research (IFW), Dresden — Motivated by the recent discovery of superatom states in C$_{60}$[1], we studied the electronic structures of an endohedral fullerene, Sr$_2$N@C$_{80}$, adsorbed on copper surface by LT-STM experiment and DFT calculation. Both experimental and calculated results show that superatom states also exist in Sr$_2$N@C$_{80}$. Different from the C$_{60}$, the encapsulated cluster (Sr$_2$N—) in Sr$_2$N@C$_{80}$ distorts the nearly-spherical potential of the carbon cage, making the atom-like orbitals look asymmetric in the STM images. The adsorbed molecules exhibit various shapes of superatom orbitals due to the different orientation of the Sr$_2$N cluster on the surface. When two molecule form the dimer, we were able to study the strong intermolecular hybridization which perturbs the penetration induced by the inside clusters, making all the dimers to have similar H$_2$-like molecular orbitals with clear bonding and anti-bonding characteristics. [1] Min Feng, Jin Zhao, Hrvoje Petek Science, 320, 359, 2008.

This research was sponsored by the Keck Foundation and DOE.

10:12AM V24.00010 Isotropic Wave Function Delocalization in C$_{60}$ Molecular Assemblies, MIN FENG, JIN ZHAO, HRVOJE PETEK, University of Pittsburgh — Electronic wave function delocalization in a molecular material is highly surprising. Here, we describe a new paradigm of strong intermolecular hybridization of a hollow core-bound molecular state in C$_{60}$ assemblies. In 1D C$_{60}$ wire and 2D C$_{60}$ island, LT-STM revealed extensive, isotropic wave function delocalization at energy above 3.5eV, in contrast with the poor intermolecular wave function overlap of the π-molecular orbitals. DFT indicates that a new kind of molecular orbital, which is derived from the central potential of the hollow cage shape of C$_{60}$, is responsible for this NFE like wave function delocalization. This central potential derived from the screening interaction and gives rise to s, p, d, etc., symmetry orbitals, which we dub the superatom molecular orbitals (SAMOs). Studies show how these atomlike orbitals hybridize into H$_2$ moleculer orbitals and p symmetry bonding/antibonding orbitals of C$_{60}$ dimers, and for larger aggregates, with alkali atom-like NFE dispersions. As a common consequence of a hollow topology, we expect that similar SAMO states will exist in other molecules derived by wrapping and rolling molecular sheets into hollow cages and nanotubes.

10:24AM V24.00011 First-principles calculation of electronic structures of new C$_{60}$ polymers, TAICHI KOSUGI, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo — C$_{60}$ fullerene molecules form fcc crystalline structure at an ambient pressure and temperature. It has been both theoretically and experimentally confirmed that this structure undergoes phase transitions into various structures at high temperatures and high pressures. Yamanaka et al. experimentally found that the individual C60 molecules in fcc structure, which are weakly bonded via van der Waals interactions, are connected to its neighbouring molecules under high temperature and high pressure, leading to the two-dimensional layered insulating rhombohedral polymer 2D-r, which is further polymerized under higher pressure and temperature into the three-dimensional polymer 3D-r. We searched for a new rhombohedral structure of C$_{60}$ polymer using ab initio calculations of the electronic structures and compared it with the experimentally observed data. In addition we quantitatively analyzed how the difference between the chemical bondings in these structures affect their energetics.

10:36AM V24.00012 Role of OH Adsorption on the Properties of MRI contrast agent Gd$_3$N@C$_{80}$, VINCE ONG, SHIV KHANNA, PANOS FATOUROS, Virginia Commonwealth University, SHIV KHANNA RESEARCH GROUP COLLABORATION, PANOS FATOUROS COLLABORATION — Endohedral metallofullerenes Gd$_3$N@C$_{80}$ decorated with hydroxyl groups are now known to be excellent contrast enhancement agents for Magnetic Resonance Imaging (MRI) leading to strong relaxivity enhancements. One of the outstanding issues is the nature of OH adsorption and its effect on the properties of endohedral Gd$_3$N motif. We have carried out theoretical studies on the electronic structure and magnetic properties of the endohedral metallofullerenes functionalized with hydroxyl groups to demonstrate that the nature of OH can have significant effect on the magnetic spin density. The new findings may provide physical insight into the observed strong relaxivity enhancements.

10:48AM V24.00013 Imaging and Spectroscopy of Diamondoid-Fullerene Hybrid Molecules$^1$, J.C. RANDEL, H.C. MANOHARAN, Stanford University — Diamondoids have attracted attention as potential building blocks for nanometer-scale electronic and mechanical devices. The ability to functionalize diamondoids with various atomic and molecular groups enables customizable chemistry, as well as tunable electronic properties. Recently, the library of realizable functional groups has expanded beyond a few atoms, and now includes C$_{60}$ fullerene. This addition provides a novel opportunity to study a material that combines the sp$^2$ and sp$^3$ forms of carbon bonding in one hybrid molecule. We investigate these molecules using scanning tunneling microscopy and spectroscopy. We find that thin films of the molecules pack in a well-ordered lattice on Au(111), and report on spectral measurements with single-molecule resolution. We comment on the connection between strong features in these electronic structure measurements and the nature of electron transport through single hybrid molecules.

We thank J. E. P. Dahl, R. M. Carlson, and P. R. Schreiner for materials and synthesis, and acknowledge support from DOE and the Chevron Corporation.
Thursday, March 19, 2009 8:00AM - 11:00AM –
Session V25 DMP: Focus Session: Graphene XIII: Spectroscopic and Transport Properties 327

8:00AM V25.00001 Charged Impurity Scattering in Graphene induced by adsorption of calcium, MASAHIRO ISHIGAMI, JYOTI KATOCH, Department of Physics, University of Central Florida — We have measured the impact of charged impurity scattering induced by adsorbed calcium atoms on the transport properties of graphene sheets. We vary the density of adsorbed atoms on the surface of graphene-based devices which are otherwise devoid of any surface adsorbates in ultra high vacuum environment. We will discuss the impact of calcium atoms on the charge carrier mobility, gate-dependent conductivity and minimum conductivity in comparison with earlier measurements performed using potassium.

8:12AM V25.00002 Current-Phase Measurements in Single Layer Graphene, CESAR CHIALVO, ION MORARU, DANIEL BAHR, NADYA MASON, DALE VAN HARLINGEN, Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign — The current-phase relationship (CPR) of a Josephson junction can provide key information about the microscopic processes that make up a supercurrent. However, CPR has not been previously measured in graphene. We have successfully fabricated a variety of Josephson junctions containing single-layer graphene as a weak link, and with different junction width to length ratios. We present results of measurements based on a phase-sensitive SQUID technique, where we determine the supercurrent amplitude and phase, as well as a possibly anomalous shape of the CPR.

8:24AM V25.00003 Landau level spectroscopy of Dirac fermions in multilayer epitaxial graphene and graphite, MAREK POTEMSKI, Grenoble High Magnetic Field Laboratory, CNRS — The results of magneto-absorption studies of epitaxial multilayer graphene on SiC and of graphite will be presented. The talk will be focused on inter Landau level transitions characteristic of electronic states with Dirac-like dispersion relations which are distinctive of graphene but persist in multilayer epitaxial graphene and are also present at the H-point of bulk graphene. The high energy limits of the Dirac-cone in epitaxial graphene will be discussed from experiments carried out in the near-infrared spectral range. Probing the nearest vicinity of the Dirac point with far-infrared light will be testified. An exceptional quality of essentially neutral multilayers of graphene on SiC (low temperature carrier mobilities ~250 000cm²/Vs) will be discussed from cyclotron resonance absorption resonance. This resonance will be shown to persist up to room temperature with negligible changes of the width which indicates no relevant thermally activated scattering process in this material.

9:00AM V25.00004 Charged Impurity Scattering in Bilayer Graphene, SHUDONG XIAO, JIANHAO CHEN, ELLEN D. WILLIAMS, MICHAEL S. FUHRER — Materials Research Science and Engineering Center and Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD, 20742, USA We have examined the impact of charged impurity scattering on the charge carrier transport in bilayer graphene in ultra-high vacuum (UHV) at low temperatures. Bilayer graphene sheets are experimentally exfoliated on Si/SiO₂ substrates, and the number of layers is verified by micro-Raman spectroscopy. Charged impurity density is varied over a wide range (up to 2x10¹⁵ cm⁻²) by deposition of potassium atoms on clean bilayer graphene in UHV. At a gate-induced charge carrier density of 4.3 x 10¹² cm⁻², the mobility is inversely proportional to the charged impurity density \( \mu = 5 \times 10^{15} \text{ V}^{-1}\text{s}^{-1}\text{cm}²/\text{V}_{\text{imp}} \). Surprisingly, the coefficient relating \( \mu \) to \( 1/|n_{\text{imp}}| \) has a similar magnitude to that for single-layer graphene, indicating a similar strength for charged impurity scattering at this carrier density. The magnitude of charged impurity scattering, as well as the implications for the source of disorder in undoped bilayer graphene, will be discussed in the context of Boltzmann transport theory.

9:12AM V25.00005 Band structure asymmetry of bilayer graphene revealed by infrared spectroscopy, ZHIQIANG LI, University of California, San Diego, ERIK HENRIKSEN, ZHIGANG JIANG, ZHAO HAO, Lawrence Berkeley National Laboratory, MATT ZHANG, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, PHILIP KIM, Columbia University, HORST STORMER, Columbia University/Bell Labs, DIMITRI BASOV, University of California, San Diego — We report on infrared spectroscopy of bilayer graphene integrated in gated structures. The dominant feature of the optical conductivity is a resonant peak due to interband transitions between the two conduction bands or two valence bands. Both the frequency and the voltage dependence of the peak show a significant asymmetry upon electrostatic doping of electrons and holes. We show that this finding arises from a marked asymmetry between the valence and conduction bands, which is mainly due to the inequivalence of the two sublattices within the graphene layer and the interlayer coupling. From the conductivity data, the energy difference of the two sublattices and the interlayer coupling energy are directly determined.

9:24AM V25.00006 On the dynamical and dc conductivity of graphene, TOBIAS STAUBER, University of Minho — It was only recently shown that a simply-observable quantity as the optical transparency of suspended graphene is defined solely by the fine structure constant [1]. In this talk, I will give the theoretical explanation to this experiment, i.e., show that even in the visible-optics regime the corrections to the Dirac cone approximation are small (a few percent) and the effect of next-nearest neighbor hopping is negligible [2]. I will also discuss the infrared conductivity of graphene on a substrate where electron-phonon and impurity scattering become important [3]. Finally, I will comment on the still unsettled question of dc conductivity in graphene and discuss - apart from Coulomb scattering - an alternative scattering mechanism based on midgap states [4].

10:00AM V25.00007 Thermoelectric and Magnetothermoelectric Transport Measurements of Graphene, YURI M. ZUEV, Applied Physics, Columbia University, WILLY CHANG, PHILIP KIM, Physics, Columbia University — We investigated the electronic, thermoelectric, and magnetothermoelectric transport properties of graphene as a function of temperature and carrier density. Microfabricated heater and thermometer electrodes were used to simultaneously measure conductance and thermoelectric power (TEP) of graphene in the temperature range of 4-300K. Graphene exhibits both positive and negative values of TEP, with a peak value on the order of kBT/|e|, when the Fermi energy is below and above the charge neutrality point, respectively. A quantitative comparison of the conductance and TEP can be made using the semiclassical Mott relation. We observed an excellent quantitative agreement between the measured TEP and the Mott relation based on the mesoscopic two terminal conductance in the low temperature regime (T < 30K). At higher temperatures, the Mott relation employing the local conductivity is necessary. Upon applying magnetic field, the magneto-thermopower exhibits characteristic oscillations in accordance with the Shubnikov-de Hass oscillations in conductance. In the quantum Hall regime at high B field, we observed the quantizing transverse and longitudinal thermopower components which are also in good agreement with the generalized Mott relation, except near the charge neutral Dirac point.
10:12AM V25.00008 Piezoresistivity of graphene-based thin films, RAHUL RAVEENDRAN NAIR, K.S. NAVOSELOV, DA JIANG, SOREN NEUBECK, LEONID PONOMARENKO, A.K. GEIM, School of Physics and Astronomy, University of Manchester — Large-scale production of graphene films is of particular interest because of graphene’s extraordinary electronic, mechanical and optical properties. We report the properties of graphene films produced by spraying or spinning of a graphene suspension obtained by ultrasonic cleavage of graphene in organic solvents, the route that does not involve graphene oxide [1]. Wafer-scale uniform films of overlapping submicron graphene crystallites were made on transparent substrates and exhibited sheet resistivity of a few kΩ with more than 80% transmission with respect to white light. Electric measurements and Raman studies suggest that the films are p-doped. In particular, we have investigated the piezoresistive effect in such films by depositing them on flexible plastic substrates. Fully reversible changes in the resistance were observed as a function of strain that could exceed 8% before the films started loosing their continuity. The piezoresistive gauge factor was up to ~30 for our films. [1] Peter Blake et al., Nano Lett. 2008, 8,1704-1708.

10:24AM V25.00009 Graphite in the bi-layer regime: in-plane transport, CHUN HUNG LUI, KIN FAI MAK, MATTHEW SFEIR, JAMES MISEWICH, TONY HEINZ, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 — Bilayers of graphene have attracted intense interest because of the possibility of tuning of their band gap by the application of a perpendicular electric field [Tsaiuke Ohta et al. Science 313, 951 (2006)]. Indeed, such gate electric fields induce both 1) tuning of the chemical potential and 2) modification of the bilayer electronic structure by the development of potential difference across the two layers. These effects have significant consequences for the infrared absorption, which probes the interband transitions, of bilayer samples. We have examined these issues by measuring the evolution of the optical conductivity (for photon energies of 0.2 - 0.8 eV) of graphene bilayer field-effect transistors constructed with a transparent top gate. The infrared absorption shows a significant and reproducible variation with gate voltage. The behavior for positive and negative gate voltages reveals an electron/hole asymmetry, reflecting corresponding differences in the band structure. The role of the development of a band gap in these structures and the effect of electrostatic screening will be discussed. Work supported by the AFOSR.

10:36AM V25.00010 Tuning the Infrared Absorption of a Bilayer Graphene Field-Effect Transistor, WEIGANG WANG, KO MUNAKATA, MICHAEL ROZLER, FRANCOISE KIDWINGIRA, MALCOLM BEASLEY, Stanford University — Scanning tunneling potentiometry (STP) is a local transport measurement that was demonstrated some time ago, but has only recently been developed in a generally useful form. Near equilibrium, STP measures the electrochemical potential along a sample surface with near nanometer spatial resolution. With our newly developed STP system, we report preliminary results on few-layer graphene at room temperature and 4.2K. Room temperature STP data show a constant drift in the electric properties. At low temperature, however, our data show no such drift. Possible evidence for Landauer resistivity dipoles will be presented. Work supported by the AFOSR.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V26 DMP: Focus Session: Graphene XIV: Magnetism and Bilayers 328

8:00AM V26.00001 Defect-induced magnetism in graphene nanoflakes, E. MARTINEZ-GUERRA, M.E. CIFUENTAS-QUINTAL, R. DE COSS, Departamento de Física Aplicada, Cinvestav-Merida, Yucatan, Mexico — The interaction between electron spin and the magnetic moments of vacancies in graphene nanoflakes can open new opportunities for spintronic and quantum computation. In that direction, we have studied the magnetic properties of graphene nanoflakes (GnFs) with a simple vacancy. Using a pseudopotential LCAO method with a Generalized Gradient Approximation (GGA) for the exchange-correlation energy functional, in particular, we have calculated the magnetic moment of graphene nanoflakes of different diameters with a simple vacancy. We have found that the total spin-polarization of the graphene nanoflakes with a simple vacancy decreases as the diameter increases. In particular, we show that the vacancy induces the appearance of a midgap state at Fermi level. Thus, the spin degeneracy is broken, being only one of the spin channels of the midgap state occupied, the other being empty. This feature could be exploited for future spintronic applications. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 83604.

8:12AM V26.00002 Magnetism in Nanopatterned Graphene and Graphite Film, LI CHEN, DECAI YU, ELISABETH LUPTON, FENG LIU, University of Utah — We report first-principles calculations of magnetic properties of nanopatterned graphene-based nanostructures (GNBs) and nanopatterned graphite films (NGPFs). We introduce a simple geometric rule to design several novel magnetic GNBs: 6D FM nanodots with the highest possible magnetic moments, 1D FM nanoribbons, and 2D magnetic superlattices, whose predicted ground-sate magnetic ordering is confirmed by first-principles calculations. Furthermore, we show that nanopatterned graphite films (NGPFs) can exhibit magnetism similar to GNBs. In particular, graphite films with patterned nanoscale triangular holes and channels with zigzag edges all have ferromagnetic ground states.

1The work is supported by DOE.

2Current Address: Linyi Normal University,China

8:24AM V26.00003 Tunable band structure in double gated trilayer graphene, MONICA CRACIUN, SAVERIO RUSSO, MICHISAYA YAMAMOTO, Department of Applied Physics, The University of Tokyo, Japan, JEROEN OOSTINGA, ALBERTO MORPURGO, DPMC & GAP, University of Geneva, Switzerland, SEIGO TARUCHA, Department of Applied Physics, The University of Tokyo, Japan — graphene based materials are promising candidates for nano electronic applications. It is currently unclear which layer thickness is better suited for a given application, as only the properties of monolayers and bilayers have been investigated systematically. For the optimization of future devices, it is important to understand how the electronic properties of graphene based materials evolve from Dirac particles, in monolayer, to massive particles in bulk graphite. We experimentally address this question by investigating trilayer graphene, the thinnest few layer graphene system in which all the parameters determining the band structure of graphite are first found. Contrary to monolayer and bilayer (which are both zero gap semiconductors), we find that trilayer is a semimetal with a finite overlap of conduction and valence bands. We show that the low energy band structure of trilayer graphene can be tuned by a large amount by means of an external perpendicular electric field, achieving 100% change in band overlap a property not known to occur in any other semimetal.
We address this controversy by providing clear experimental evidence that metal free carbon can be ferromagnetic at room temperature using dichroism x-ray absorption spectro-microscopy. For this purpose we acquired soft x-ray microscopy images of magnetic structures on a thin carbon film that have been produced by irradiation with a focused 2.25MeV proton beam. Our element specific magnetic probe shows no indication of magnetically ordered Fe, Co or Ni impurities in these samples. Combination of the microscopy data with element specific spectroscopy and hysteresis measurements shows furthermore that only the carbon z-electronic states contribute to the long range ferromagnetic order of the sample.

The recent discovery that the application of an external electric field induces a band gap opening in doped bilayer graphene, in presence of different bottom and top gate, in particular, the dependence of the band gap on the doping, on the average external electric field and temperature has been analysed. We find that our ab-initio results differ with respect to those obtained with standard Tight Binding (TB) calculations [2]. In particular, we show important charge effects, which are crucial for the description of the electronic properties of bilayer graphene, and which are not included in TB models. Moreover, we compare our results with experimental measurements of the band gap, cyclotron mass and work function. [1] Ohta et al., Science v.313, 951 (2006). [2] Castro Neto et al., Phys. Rev. Lett. v.99, 216802 (2007).

This work is supported by the DOE under DE-FG02-07ER46453 through the Frederick Seitz Materials Research Laboratory.
The measurement of protein interaction provides an intriguing opportunity for Atomic Force Microscopy (AFM)-based force measurements. The AFM has the advantage that it is relatively easy to use and widely available. However, the interpretation of the force data is lagging behind the experimental capabilities of the technique. In this talk, I will present some recent results of rupture force measurements between two proteins, and discuss our efforts to interpret the resulting data in terms of the underlying energy landscape. We performed measurements on matrix metalloproteinases and their natural inhibitors at pulling speeds ranging over 3 orders of magnitude (30-48000 nm/s). However, we found that commonly used theory to interpret such data is inadequate and does not capture the physics of the problem. Consequently, data analysis based on such theories leads to highly erroneous results. We will discuss our attempts to improve the theory and present parameters extracted from the data that reflect the underlying energy landscape of the studied protein-protein interaction.

10:12AM V26.00012 Plasmon Dispersion and Damping in Electrically-isolated Two-dimensional Charge Sheets, YU LIU, ROY WILLIS, Pennsylvania State University — Using high resolution reflection electron-energy-loss-spectroscopy (HREELS), we compare experimental results for the wavevector-dependent behavior of plasmons in a graphene nanoribbon on SiC(0001) with that due to a filled band of surface states on semiconducting silicon. There are significant differences in behavior between the two systems, and the behavior predicted for a classical two-dimensional sheet of electrons. In particular, the damping increases with wavevector independent of any obvious inelastic scattering channel. The results illustrate the importance of finite-momentum, non-local potential effects for the dynamical behavior of electrically-isolated charge sheets.


10:24AM V26.00013 ABSTRACT WITHDRAWN —

10:36AM V26.00014 Edge Phonons of Graphene from Tight-Binding, DANIEL FINKENSTADT, U.S. Naval Academy, Physics Department, N. BERNSTEIN, D. GUNLYCZE, M.J. MEHL, U.S. Naval Research Laboratory, Washington, DC — Edge-states in graphene can affect the band-gap and carrier group velocities in narrow (< 5 nm) graphene nanoribbons. As a first, tight-binding approximation from simple nearest-neighbor hopping, it is shown that armchair nanoribbons have large band-gaps compared to zigzag nanoribbons, which are metallic, unless certain crucial effects are included in the calculation, e.g. magnetic, quasiparticle, charge-self-consistent, and/or relaxation-based degeneracy lifting. All of these effects open a small band gap, and the interplay between relaxation and electronic structure may be examined by calculating the edge phonons of graphene. To this end, we expand on our previous, all-neighbor tight-binding Hamiltonian [Phys. Rev. B 76, 121405(R) (2007)] and include charge self-consistency at the edge of a zigzag nanoribbon. By allowing charge transfer and structural-relaxation at zigzag edges, we are able to remove imaginary phonons and verify the opening of a small band-gap in zigzag ribbons, which is characterized by the phonon-density-of-states and normal modes of carbon-hydrogen edge bonds. These calculations are relevant to ribbons cut along non-ideal directions, as well, and we will discuss edge-disorder.

1Supported by the Office of Naval Research, National Research Council.

10:48AM V26.00015 Optical Conductivity and quasiparticle properties of Bilayer graphene, YAFIS BARLAS, KUN YANG, NHMFL, Tallahassee, FL — The low energy properties of Bernal stacked bilayer graphene can be adequately described by chiral quasiparticles exhibiting a Berry phase of 2π with a parabolic dispersion. When the Fermi energy lies at the neutrality point the Fermi surface consists of a pair of points where dominant inter-band excitations determine the effect on electronic correlations. The particle-hole continuum due to the inter-band excitations is given by Ω > q²/(4m) in frequency-momentum space. The full wavevector and frequency dependent polarization bubble and optical conductivity is calculated within the RPA. We also calculate the quasiparticle properties for short-ranged interactions and comment on the breakdown of Fermi liquid theory.

Thursday, March 19, 2009 8:00AM - 10:48AM — Session V27 GIMS: Focus Session: Emerging Scanning Probe Microscopy Methods for Biological Applications 329

8:00AM V27.00001 Kinetic parameters of association and dissociation between single molecules measured by single-molecule force spectroscopy, BORIS AKHREMITCHEV, Duke University — This presentation is focused on development of experimental scanning probe microscopy (SPM) approaches to quantify kinetic parameters of association and dissociation between receptor-ligand pairs. The potential of mean force (pmf) between interacting molecules is quantified by single molecule force spectroscopy (SMFS) approach. In SMFS molecules are allowed to interact and form molecular bond. Consequent measurements of rupture forces are used to characterize the attractive part of the pmf by extracting the distance from the equilibrium to the transition state, the rate of dissociation at no force and the activation energy. Factors affecting accuracy of the measured kinetic parameters are discussed including effects of the polymeric tether stiffening and possible contribution of non-single molecule events to the statistics of rupture forces. The developed SMFS method accounts for pertinent systematic errors and is tested using specific biotin-streptavidin interactions. The measured kinetic parameters show quantitative agreement with theoretical predictions. In addition, a new single-molecule approach to measure the activation energy of association is proposed. This approach uses the dependence of the probability to form molecular bonds on probe velocity when one of the interacting molecules is tethered by a flexible polymeric linker to the AFM probe. The application of the developed method to study interactions between biomolecules is demonstrated with measurements of the activation energy of biotin-streptavidin association.

8:36AM V27.00002 Coaxial and Triaxial Atomic Force Microscope Probes for Nanoassembly, KEITH A. BROWN, JONATHAN AGUILAR, R.M. WESTERVELT, Harvard SEAS and Physics — We present a technique for the controlled three dimensional assembly of nanoscale objects using a modified atomic force microscope (AFM) probe. A conducting AFM probe is coated with alternating insulating and metal layers then etched at the tip to expose coaxial electrodes. The fabrication allows freedom to specify the size of the tip and therefore the length scale of objects to manipulate. An RF voltage is applied to the electrodes to trap objects at the tip with dielectricphoresis (DEP). The object may be released when it has been moved to the desired location by turning off the field. We present a two electrode coaxial configuration capable of positive DEP and a three electrode triaxial configuration for negative DEP which holds the trapped object away from the tip to overcome the “sticky finger” problem. The integration of three dimensional assembly with the nanometer precision and force-imaging capability of an AFM creates a platform for imaging and constructing structures at the nanoscale. We describe initial experiments and fabrication.

8:48AM V27.00003 Protein bond rupture measured by AFM and the energy landscape problem, PETER HOFFMANN, ESSA MAYYAS, LINDSAY RUNYAN, Wayne State University — The measurement of protein interaction provides an intriguing opportunity for Atomic Force Microscopy (AFM)-based force measurements. The AFM has the advantage that it is relatively easy to use and widely available. However, the interpretation of the force data is lagging behind the experimental capabilities of the technique. In this talk, I will present some recent results of rupture force measurements between two proteins, and discuss our efforts to interpret the resulting data in terms of the underlying energy landscape. We performed measurements on matrix metalloproteinases and their natural inhibitors at pulling speeds ranging over 3 orders of magnitude (30-48000 nm/s). However, we found that commonly used theory to interpret such data is inadequate and does not capture the physics of the problem. Consequently, data analysis based on such theories leads to highly erroneous results. We will discuss our attempts to improve the theory and present parameters extracted from the data that reflect the underlying energy landscape of the studied protein-protein interaction.
9:00AM V27.00004 AFM method to detect differences in adhesion of silica beads to cancer and normal epithelial cells. IGOR SOKOLOV, Clarkson University, SWAMINATHAN IYER, University of Western Australia, RAVI GAIKWAD, CRAIG WOODWORTH, Clarkson University — To date, the methods of detection of cancer cells have been mostly based on traditional techniques used in biology, such as visual identification of malignant changes, cell growth analysis, specific ligand-receptor labeling, or genetic tests. Despite being well developed, these methods are either insufficiently accurate or require a lengthy complicated analysis. A search for alternative methods for the detection of cancer cells may be a fruitful approach. Here we describe an AFM study that may result in a new method for detection of cancer cells in vitro. We use atomic force microscopy (AFM) to study adhesion of single silica beads to malignant and normal cells cultured from human cervix. We found that adhesion depends on the time of contact, and can be statistically different for malignant and normal cells. Using these data, one could develop an optical method of cancer detection based on adhesion of various silica beads.

1Partial support from Nano-Bio Laboratory (NABLAB), Clarkson University and NSF CCR-0304143 is acknowledged.

9:12AM V27.00005 Rapid Cellular Identification by Dynamic Electromechanical Response; VLADIMIR REUKOV, MAXIM NIKIFOROV, ALEXEI VERTEGEL, GARY THOMPSON, STÉPHEN JESSE, SERGEI KALININ, OAK RIDGE NATIONAL LABORATORY TEAM, CLEMSON UNIVERSITY TEAM — Quick and reliable identification of individual prokaryotic organisms and cellular types is of utmost importance for various applications. A number of strategies for cellular identification are currently used to meet this challenge. All of the existing techniques require culturing bacteria prior to measurement, which increases the time needed for experimentation and analysis considerably. Here, we report on a method for rapid cellular identification and mapping using the detection of broadband electromechanical response. Electromechanical spectra from M. Lysodeikits and P. Fluorescens deposited on PLL-coated mica were collected over wide frequency range. Principal component analysis of the spectra bundled with neural network analysis provides a robust algorithm for identification of the cellular organisms based on their electromechanical properties.

1This Research at Oak Ridge National Laboratory’s Center for Nanophase Materials Sciences was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

9:24AM V27.00006 Simultaneous Nanomechanical and 3d Optical Microscopy: Cellular Distortions and Structural Dynamics; BRYAN HUEY, University of Connecticut, Institute of Materials Science — Combined SPM and Optical systems are increasingly used to study biological structures, including living cells. Here, an AFM is employed to expose cells to foreign bodies and biochemicals, and to measure the resulting attractive and repulsive forces exerted by the cell. 3d optical fluorescence measurements are simultaneously performed revealing distortions and/or restructuring of the cell, membrane, actin cytoskeleton, etc. The work focuses primarily on MH-S cells (mouse lung macrophages) transfected with GAP-43 GFP to identify cell membranes and/or mCherry Actin to identify cytoskeleton dynamics. During standard AFM, optical-cross sections reveal drastic cell distortions up to 50 percent. The viscoelastic response of the cells to nanoNewton induced forces by Silica and Polystyrene beads is also quantified via Structural Recovery After Probing (STRAP), which monitors the rate of cellular recovery following nanodentation.

1Supported by NSF-Nanobiomechanics (#0626231).

10:00AM V27.00007 Spectral Oscillations in Backscattering of Light from a Biological Cell; ALEXANDER HEIFETZ, Argonne National Laboratory, ALEXANDER PATASHINSKI, VADIM BACKMAN, Northwestern University — Based on general electrodynamics principles, we provide an explanation for spectral oscillations in the intensity of visible light elastic backscattering from a live epithelial biological cell. We suggest that the source of spectral oscillations in backscattering from a cell is the nucleus, which is a spheroidal particle several times larger than the incident wavelength, and has a sharp boundary. Because of the small optical contrast of the nucleus relative to surrounding cytoplasm, contribution of single scattering to the overall signal is comparable to that of multiple scattering. We show that the high frequency spectral oscillations in backscattering are due to single scattering, which can be obtained in the first Born approximation. Multiple scattering effects result in slow envelope spectral oscillations. We expand the Mie backscattering cross-section of a uniform sphere in power series to show that the equivalence between the first order Mie backscattering and first Born series.

1American Cancer Society & Canary Foundation.

10:12AM V27.00008 Single-molecule detection of near-infrared phthalocyanine dyes; YOU LI, BRIAN CANFIELD, LLOYD DAVIS, University of Tennessee Space Institute — The major advantage associated with near-IR monitoring is the fact that few compounds exhibit intrinsic fluorescence in this region of the spectrum. Phthalocyanine dyes provide excellent photostability and hence are an attractive candidate for fluorescence bioassay applications. However, because of their small Stokes shifts, non-standard methods are needed for separation of fluorescence from scattered laser light. We have developed a custom confocal microscope that uses a low-cost laser diode operating at 665.8 nm for sample excitation and an angle-tuned Raman notch filter to block scattered laser radiation and provide high-throughput of fluorescence. Also, a diffraction grating is used to isolate the laser excitation wavelength from the broad background luminescence of the laser. We have used the system to observe photon bursts from single molecules of zinc phthalocyanine fluorophores in an ethanol solution. The autocorrelation function of the photon trace provides a measure of the signal-to-noise ratio. We also discuss ongoing experiments to characterize the limits of detection of near-infrared fluorophores in aqueous solution using the microscope.

10:24AM V27.00009 Chemical Recognition Tunneling via Hydrogen Bond; JIN HE, the Biodesign Institute, Arizona State University, SHUAI CHANG, LISHA LIN, SHUO HUANG, ASHLEY KIBEL, MYEONG LEE, PEIMING ZHANG, OTTO SANKEY, STUART LINDSAY, Arizona State University — Hydrogen bonds enhance electron tunneling rates over vacuum tunneling as well as making chemically selective attachments to target molecules when patterns of donors and acceptors match. This raises the possibility of a completely new approach to transducing chemical information into electrical signals, based on forming an electrical circuit via a target molecule that bridges a gap between two electrodes by means of hydrogen bonding. Hydrogen-bond sensitive contrast has recently been demonstrated in scanning-tunneling microscope (STM) images of DNA bases. In this presentation, I will first show that the tunnel-current vs. distance decay curves acquired by STM change shape with the number of hydrogen bonds mediating an interaction. [1] Base composition of DNA oligomers can be resolved by this method. Further studies demonstrate that these tunnel-current decay signals can be used to count the number of hydrogen bonds in interactions between DNA bases and related compounds. The signals are partially mechanical in origin, reflecting the tensile strength of a tunnel junction held together with hydrogen bonds.

10:36AM V27.00010 Nanoscale Properties of Neural Cell Prosthetic and Astrocyte Response, D.A. FLOWERS, Wayne State University, MI, V.M. AYRES, Michigan State University, R. DELGADO-RIVERA, Rutgers University, NJ, I. AHMÉD, S.A. MEINERS, University of Medicine and Dentistry of New Jersey — Preliminary data from in-vivo investigations (rat model) suggest that a nanofiber prosthetic device of fibroblast growth factor-2 (FGF-2)-modified nanofibers can correctly guide regenerating axons across an injury gap with aligned functional recovery. Scanning Probe Recognition Microscopy (SPRM) with auto-tracking of individual nanofibers is used for investigation of the key nanoscale properties of the nanofiber prosthetic device for central nervous system tissue engineering and repair. The key properties under SPRM investigation include nanofiber stiffness and surface roughness, nanofiber curvature, nanofiber mesh density and porosity, and growth factor presentation and distribution. Each of these factors has been demonstrated to have global effects on cell morphology, function, proliferation, morphogenesis, migration, and differentiation. The effect of FGF-2 modification on the key nanoscale properties is investigated. Results from the nanofiber prosthetic properties investigations are correlated with astrocyte response to unmodified and FGF-2 modified scaffolds, using 2D planar substrates as a control.

Thursday, March 19, 2009 8:00AM - 11:00AM — Session V28 FLAP: Focus Session: Graphene Device and Applications III 330

8:00AM V28.00001 Graphene field-effect transistors for RF applicatons1, KENNETH SHEPARD, Columbia University — There has been growing interest in graphene as a replacement for III-V materials in MMIC applications because of its high mobility, its potential for high saturation velocity, and its nearly perfect two-dimensional electrostatics. We present results from the first experimental high-frequency measurements of graphene field-effect transistors (GFETs), demonstrating an fT of 14.7 GHz for a 0.5-µm-length device with a 30-nm-thick HfO2 gate-poly. Despite lOn/loff ~7, high transconductances (>533 µS/µm) and current saturation are achieved. We present detailed measurement and analysis of velocity saturation in GFETs, demonstrating the potential for velocities approaching 10^6 cm/sec and the effect of an ambipolar channel on current-voltage characteristics. We find that the saturation velocity is sheet-carrier dependent and limited by interfacial phonon scattering from the SiO2 substrate upon which the graphene is fabricated.

1This work was supported by the C2S2 Center of the Focus Center Research Program.

8:36AM V28.00002 Tunable spin-polarized terahertz excitations in graphene nanoribbons1, JUN-QIANG LU, University of Puerto Rico, XIAOGUANG ZHANG, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — Graphene nanoribbons have an energy gap that is tunable from zero to terahertz (THz) regime by an external gate field. The indirect energy gap in a nanoribbon of infinite length, however, is unsuitable for optical excitations. We report a theoretical investigation of such nanoribbons with a finite, nanoscale length. We show that such nanoribbons can be excited optically and exhibit unique electronic excitations in the THz regime. The results unveil THz radiation-induced edge standing spin waves with different wavelengths at the two edges and a resonant frequency that can be controlled by an external gate voltage, opening the possibility of THz “opto-spintronic” applications.

1Work at CNMS at ORNL sponsored by Division of User Facilities, Office of Basic Energy Sciences, US Department of Energy.

8:48AM V28.00003 THz Emission from Graphite Surfaces, CHEN XIA, JIE SHAN, Physics Department, Case Western Reserve University — Graphite formed by Van der Waals force between adjacent graphite sheets has been studied for more than six decades due to its relatively simple quasi-two-dimensional structure. Lately, because of its close relationship to carbon nanotubes and new physics originating from graphite’s linear excitations spectrum and the 4-fold degeneracy of the electronic states, graphite materials have attracted much of research attention. However, still little is known about the high-frequency transport properties of these materials. In this work, we investigate graphite materials in THz regime by THz emission spectroscopy. Picosecond THz pulses were observed from a highly oriented pyrolytic graphite (HOPG) surface when it was illuminated by intense ultrafast optical pulses at an oblique angle. The emission was mostly p-polarized and increased linearly with pump fluence. Several potential mechanisms for the emission including surface nonlinearities will be discussed in the talk.

9:00AM V28.00004 Low - Frequency Noise in Graphene Transistors2, GUANXIONG LIU, QINGHUI SHAO, DESALEGNE TEWELDEBRHAN, ALEXANDER BALANDIN, Nano-Device Laboratory, Electrical Engineering, University of California Riverside, Riverside, CA, SERGUEI ROUMYANTSEV, MICHAEL SHUR, Center for Integrated Electronics, Electrical, Computer and Systems Engineering, Rensselaer Polytechnic Institute, Troy, New York — We present the results of the experimental investigation of the low-frequency noise in three-terminal bilayer graphene devices. The quality of graphene layers has been verified with micro-Raman spectroscopy. Back-gated devices were fabricated using electron beam lithography and evaporated. The back-gate was used to adjust electrical conductivity through the graphene layer placed on top of Si/SiO2 substrate. The charge neutrality point for examined devices was ~10 V. The noise spectral density was rather low (on the order of ~10E−21−10E−22 A2/Hz at frequency of 1 kHz). The noise reveals generation-recombination (G-R) bulges. Presence of G-R bulges and deviation from the 1/f spectrum suggest that the noise is of carrier-number fluctuation origin due to carrier trapping by defects [1]. The low values of the low-frequency noise add validity to the proposed electronic applications of graphene.

2This work at UCR was supported in part by DARPA SRC FENA and IFC.

9:12AM V28.00005 Environmental Effects on 1/f Noise in Graphene and CNT Based Devices3, BRETT R. GOLDSMITH, YE LU, ZHENG TANG LUO, A.T. CHARLIE JOHNSON, University of Pennsylvania — Graphite related materials such as carbon nanotubes, graphene and graphene oxide show promise for future electronic and chemical sensor applications. Nanotubes and graphene, in particular, have been shown to make exquisitely sensitive chemical sensors. Due to their low carrier density, the 1/f noise in these nanomaterials is very high. Understanding the cause of this noise is particularly important for chemical sensing applications, and the noise common to these materials may be one barrier to current practical success for graphitic sensors outside the lab. We have compared the noise power spectral density (PSD) of these three materials in different chemical environments and at different temperatures. This information should play a key role in guiding the development of future sensing devices as well as helping to illuminate the atomic scale interactions which lead to enhanced or suppressed 1/f noise in graphitic materials.

3This research was supported by the Intelligence Community Postdoctoral Research Fellowship Program award number HM1582-07-1-2014.

9:24AM V28.00006 ABSTRACT WITHDRAWN —
10:00AM V28.00007 Progress towards graphene as a quantum-limited electro-mechanical resonator

R. G. KNOBEL, A. CHIA, Queens University, Department of Physics — With its high stiffness, low density and relatively simple fabrication, graphene promises to be an ideal system for exploring the quantum limits of mechanical measurements. In particular, electronic transport through a graphene sheet suspended over an electrode can be strongly modulated by vibrations of the sheet — whether through the standard field effect which changes the carrier density in the sheet, or through modification of the Coulomb blockade in quantum dots formed in the sheet. In this work we present the novel fabrication scheme we are using for this work, which involves exfoliation and identification of single-layer graphene sheets on a PMMA layer above a silicon substrate, cross-linking of the PMMA to form supports for the graphene and metal electrodes, and subsequent lithography to form electrodes. Raman scattering measurements before and after patterning confirm the single-layer nature of the graphene, and preliminary low-temperature transport measurements show the feasibility of this system for quantum-limited sensitivity of resonant motion of the sheet.

1Current address: McMaster University, Department of Engineering Physics

10:12AM V28.00008 Developing resonant tunneling devices based on graphene

ERIC YU, SANDIP TIWARI, Department of Electrical and Computer Engineering, Cornell University, DEREK STEWART, Cornell Nanoscale Facility, Cornell University — We present an ab-initio study of the electronic properties of patterned graphene structures as candidate resonant tunneling devices. We consider graphene nanoribbons that have been modified with one or more narrow constrictions or patterned with periodic nanoscale antidotes[1]. Specifically, we focus on semi-metallic armchair nanoribbons with narrow semiconducting regions and semi-metallic zigzag nanoribbons patterned with antidots. Using a first-principles density functional theory (DFT) approach, we investigate the induced band-gap opening and transmission coefficients. We examine how varying the lengths of the constrictions, changing the separation between dots and their sizes affect transport properties. We will also discuss I-V characteristics of these graphene structures and evaluate the possibility of a negative differential resistance in these devices. [1] T. G. Pedersen et al., Physical Review Letters, 100 136804 (2008)

10:24AM V28.00009 Coherent Graphene Devices: Movable Mirror, Buffer and Memory

L. ZHAO, Department of Physics, University of Connecticut, Storrs, CT 06269; ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138 — We theoretically report that, at a sharp electrostatic step potential in graphene, massless Dirac fermions can obtain a Goos-Hänchen-like shift under total internal reflection. Based on these results, we study the coherent propagation of the quasiparticles along a sharp graphene p-n-p waveguide and derive novel dispersion relations for the guided modes. Consequently, coherent graphene devices (e.g. movable mirror, buffer and memory) induced only by the electric field effect can be proposed.

We would like to acknowledge funding from NSF.

10:36AM V28.00010 Graphene interferometry

DANIEL GUNLYCKE, CARTER WHITE, Naval Research Laboratory — Ballistic transport calculations of graphene connected to two contacts are presented. The calculations are based on the nearest-neighbor, tight-binding approximation but are otherwise treated exactly within a Green function formalism. It is shown that under certain circumstances stable collective resonances emerge from a resonant structure that in general could be quite complicated. These collective resonances originate from a large number of non-equivalent conduction channels and are evenly spaced, except for a region close to the Fermi level. The separation between neighboring collective resonances depends to first order only on the contact separation. Their contrast, on the other hand, is affected by the width of the sample, temperature, and unevenness in the contact interfaces. Despite the existence of many potential sources that could degrade the collective resonances, these resonances could still prove to be observable experimentally.

1This work was supported by the National Research Council (NRC) and Office of Naval Research (ONR) directly and through the Naval Research Laboratory (NRL).

10:48AM V28.00011 Nanotube Films and Their Application For Mode-Locked Lasers


Thursday, March 19, 2009 8:00AM - 11:00AM
Session V29 GMAG: Correlated Electrons

8:00AM V29.00001 Emergence of spin structure in quantum wires under strong magnetic fields

GILAD BARAK, GEORG SCHUSTERTSCH, AMIR YACOBY, Harvard University. LOREN PFEIFFER, KEN WEST, Bell Labs, Lucent Technologies — We study the effects of a perpendicular magnetic field on the spin and charge structure of a quantum wire. Using momentum resolved tunneling between two parallel wires we measure the dispersion relation for different perpendicular magnetic fields. We find that as the magnetic field increases, charges with opposing spin separate in the cross section of the wire giving rise to strips of polarized and unpolarized electrons. We argue that this structure results from the exchange interaction between electrons in the wire. We discuss the applicability of these results to the structure of Quantum Hall edge states.
8:12AM V29.00002 Nonequilibrium transport in the Anderson model of a biased quantum dot1, SUNG CHAO, GUILLAUME PALACIOS, Rutgers University, ANDRES JEREZ, New Jersey Institute of Technology, CARLOS BOLECH, Rice University, PANKAJ MEHTA, Princeton University, NATAN ANDREI, Rutgers University — We derive the transport properties of a quantum dot subject to a source-drain bias by means of the Scattering Bethe Ansatz, a generalization of the traditional Thermodynamic Bethe Ansatz to open systems out of equilibrium, which allows a description of the the system in nonequilibrium steady state over the full range of its parameters. Solving the equations at zero temperature and magnetic field we present here the non-linear conductance against the bias voltage with arbitrary tunneling rate and with the gate voltage varying from the mixed valence to the Kondo regime.

1Work supported by Grant number: DMR - 0605941.

8:24AM V29.00003 Imaging the Fano lattice in the heavy fermion material URu$_2$Si$_2$ by scanning tunneling spectroscopy1, ANDREW SCHMIDT, MOHAMMAD HAMIDIAN, Cornell University, PETER WAHL, Max Planck Institut, FOCKO MEIER, Cornell University, GRAEME LUKE, McMaster University, J.C. DAVIS, Cornell University, CORNELL UNIVERSITY TEAM, MCMASTER UNIVERSITY TEAM — We present scanning tunneling spectroscopy measurements of the heavy fermion material URu$_2$Si$_2$. Two dimensional differential conductance maps of mechanically cleaved surfaces reveal a narrow Fano lineshape about the Fermi level that is pervasive across the field of view. Such a lineshape is expected whenever a discrete energy level is coupled to a continuum of levels. By fitting the spectra to a Fano function, we produce maps showing the variation of the Fano parameters across the surface.

8:36AM V29.00004 Theory of the Unusual Quasiparticle Excitations in USb$_2$, PETER RISEBOROUGH, XIAODONG YANG, Temple University — A band of long-lived quasiparticles with a renormalized dispersion relation that does not cross the Fermi surface has been observed in USb$_2$ by angle resolved photoemission measurements. The existence of a kink in the quasiparticle dispersion relation of a band that does not cross the Fermi energy is unprecedented. We show that the observed renormalization does not come from the standard theory of electron-phonon renormalizations. We consider the effect of the interband self-energy and vertex corrections as possible causes for the formation of the renormalized quasiparticles. The effect of temperature is also considered.

8:48AM V29.00005 Kink in the dispersion of f-electrons, TOMASZ DURAKIEWICZ, PETER S. RISEBOROUGH, CLIFFORD G. OLSON, JOHN J. JOYCE, PETER M. OPPENEEER, SAAD ELGAZZAR, ERIC D. BAUER, JOHN L. SARRAO, ELA GUZIEWICZ, DAVID P. MOORE, MARTIN T. BUTTERFIELD, KEVIN S. GRAHAM, LOS ALAMOS NATIONAL LABORATORY, TEMPLE UNIVERSITY, AMES LAB, UPPSALA UNIVERSITY, PAN, LLNL TEAM — Many-body interactions may result in the formation of long-lived heavy quasi-particles that exhibit kinks in their energy dispersion. Kinks are often seen in d-electron correlated systems and are attributed to many different origins, such as coupling to phonons, extended spin-fluctuations, or electron-electron correlations. We have found that the renormalization of a 5f electron band in USb$_2$ leads to the formation of a kink characterized by two distinct regions with different quasiparticle masses, peak asymmetries, lifetimes and a record-breaking small width of 3meV. The kink energy scale of 17meV originates from renormalization of a point-like Fermi surface, and is a factor of two smaller than previously measured in correlated materials.

1Research supported by DOE BES and LANL LDRD.

9:00AM V29.00006 Localized 5f antiferromagnetism in cubic UIn$_5$: $^{115}$In-NMR/NQR Study, H. SAKAI, S. KAMBE, Y. TOKUNAGA, H. CHUDO, Japan Atomic Energy Agency, Y. TOKIWA$^1$, D. AOKI$^2$, Osaka University, Y. HAGA, Japan Atomic Energy Agency, Y. ÔNUKI$^3$, Osaka University, H. YASUOKA, Japan Atomic Energy Agency — $^{115}$In nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) measurements have been performed on an antiferromagnet UIn$_5$ with the cubic AuCu$_3$-type structure. The NQR frequency ($\nu_Q$) and Knight shift (K) of $^{115}$In in UIn$_5$ have been estimated in the paramagnetic state from NMR experiments under applied field. The perpendicular component of transferred hyperfine coupling constant ($A_\perp$) has been deduced from scaled behavior of K to the static susceptibility ($\chi$). Under zero field, the observation of the NQR spectrum has led to an estimated $\nu_Q$ of 11.8 MHz at 90 K. The temperature variation of the NQR relaxation rates ($1/T_1$) far above the Néel temperature $T_N$=88 K approaches a constant value, which indicates a localized nature for the 5f- electrons in this system. On the other hand, in the antiferromagnetically ordered state at 4 K (well below $T_N$), the $^{115}$In-NQR spectrum has been scanned over frequencies ranging from ~20 to ~70 MHz under zero applied field. From the analysis of the NMR spectrum, we propose that the direction of U moments in the AF state is neither (100) nor (111), but may be (110).

$^1$Present Affiliation: Georg-August- Universität Göttingen
$^2$Present Affiliation: CEA-Grenoble
$^3$Also at: Japan Atomic Energy Agency

9:12AM V29.00007 Studies of the Ferromagnetic Superconductors URhGe and UCuGe, TRAVIS WILLIAMS, ADAM ACZEL, WEIQIANG YU, McMaster University, YASUTOMO UEMURA, JEREMY CARLO, Columbia University, TATSUO GOKO, TRUMF, JIM GARRETT, Brockhouse Institute for Materials Research, GRAEME LUKE, McMaster University — Superconductivity (SC) cannot cooperatively exist with ferromagnetism (FM) in conventional superconductors, since ferromagnetism would act to destroy Cooper pairs. Thus, in FM superconductors such as URhGe and UCuGe, a more exotic pairing type must exist. I will outline the growth and characterization of URhGe and UCuGe crystals, and our measurements of the FM and SC properties of these combined results from DC Resistivity, Bulk Magnetometry and Muon Spin Relaxation show FM properties in the samples, including a clear FM transition at 9.5K in the URhGe crystal. We will discuss our results and their implications for the nature of the SC state in these materials.

9:24AM V29.00008 Renormalization of electronic structure close to Fermi level of CeIrIn$_5$ at 20K, YINWAN LI, TOMASZ DURAKIEWICZ, JOHN J. JOYCE, KEVIN S. GRAHAM, JOHN L. SARRAO, ERIC D. BAUER, Los Alamos National Laboratory, CLIFFORD G. OLSON, Ames Lab, Iowa State University — The electronic structure of heavy-fermion super-conductor CeIrIn$_5$ is investigated at ~20K by high-resolution angle-resolved photoemission (ARPES). The low energy ARPES spectra indicate a kink near the Fermi surface within the energy scale of the order of 20meV. Existence of a kink may suggest coupling of electron to a collective boson mode of unknown origin.

$^1$Research supported by DOE BES and LANL LDRD.
9:36AM V29.00009 Interplay of magnetism and screening in the Kondo Lattice1, PIERS COLEMAN, ANDRIY NEVIDOMSKYY, Dept Physics and Astronomy, Rutgers University — An increasing body of experimental evidence suggests that frustration and the Kondo effect have complimentary roles that act together to either reduce, or completely eliminate magnetic order in heavy electron systems[1]. I will review our attempts to explore the joint effects of frustration and Kondo effect in the Kondo Heisenberg model, using the large N Schwinger boson approach[2]. These results will be discussed in the context of recent doping experiments on YbRh2Si2 [3], where an intermediate spin liquid appears to develop between the antiferromagnet and the large Fermi surface metal.

1 Supported by the Foundation for Polish Science (FNP), the Polish Research Project N202 068 32/1481, and the NSF grant DMR-0706020.

9:48AM V29.00010 Electronic band structure of Pr-based filled skutterudite antimonides1, J.W. ALLEN, B.J. KIM, RAVI S. SINGH, University of Michigan, O. KRUPIN, J.D. DENLINGER, Lawrence Berkeley National Lab, R.E. BAUMBACH, M.B. MÄPLE, UC San Diego — Filled skutterudites exhibit a wide range of strongly correlated electron phenomena including heavy fermion, superconductivity, non-Fermi liquid and quantum critical behaviors. Knowledge of the electronic structures of these materials is almost entirely from band calculations and dhvA studies. We present the first angle-resolved photoemission spectroscopy (ARPES) measurements of the filled skutterudites antimonides: PrOs4Sb12 and PrRu4Sb12. Band dispersions and Fermi surface maps of these three-dimensional materials will be discussed and compared to available LDA band structure calculations.

1Supported by the U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231), at UM (DE-FG02-07ER46379) and UCSD (FG02-04ER46105 & FG02-04ER46178).

10:00AM V29.00011 High frequency thermal transport for the 2d Hubbard model1, LOUIS-FRANCOIS ARSENAULT, SYED HASSAN, ANDRE-MARIE TRÉMBLAY, Université de Physique et RQMP, Université de Sherbrooke — In order to calculate thermal transport coefficients of correlated systems when the Boltzmann equation is not applicable, Shastry [1] has developed a new theoretical approach. Although, in this theory, quantities such as the thermopower depend only upon the one particle Green’s function, vertex corrections are included. The price to be paid is that only the high frequency limit is accessible. This may be adequate for aforementioned transport coefficients. Results for the triangular lattice t-J model and the 1d Hubbard model are already in the literature but there are no results for the 2d Hubbard model, the prototype of correlated electron systems. We thus applied the Shastry approach to the 2d Hubbard model using quantum cluster approaches that include CDMFT + exact diagonalization, Bethe’s lattice DMFT + CTQMC and CDMFT + CTQMC. Results were obtained for the thermopower as a function of temperature (T), chemical potential (μ), and band structure. Since infinite frequency is reached differently in the t-J and in the Hubbard model, our results enable us to assess the degree to which infinite frequency is related to experimental results on DC transport. [1] B. Sriram Shastry, Phys. Rev. B 73, 085117 (2006)

10:12AM V29.00012 Time evolution of excited state in the system with first-order metal-insulator transition, W. KOSHIBAE, CROSS-CORRELATED MATERIALS RESEARCH GROUP (CMRG), RIKEN, CREST, JST, N. FURUKAWA, Aoyama-Gakuin Univ., ERATO-Multiferroics, JST, c/o Dept. of Appl. Phys., Univ. of Tokyo, N. NAGAOSA, CMRG, RIKEN, CREST, JST, N. FURUKAWA, Aoyama-Gakuin Univ., ERATO-Multiferroics, JST, c/o Dept. of Appl. Phys., Univ. of Tokyo — We have studied numerically the relaxation process in the system with a first-order metal-insulator transition using the double-exchange model: $H = -t \sum \langle i,j \rangle \sum_{\sigma} (c_{i \sigma}^\dagger c_{j \sigma} + h.c.) - J_\parallel \sum \langle i \rangle \sum_{\alpha \beta} (\alpha \beta_{\alpha \beta} \delta_{\alpha \beta}) \cdot \vec{S}_i \cdot \vec{S}_ j$. The localized spin is considered to be a classical vector with a magnitude $S$. In the two-dimensional system and in the case of $S J_\parallel / t < 4$, the ground state shows a metal-insulator transition due to the change of the magnetic state. When the magnitude of the parameter $S J_\parallel / t$ is not large enough, the antiferromagnetic insulating state is stabilized because of a perfect nesting-condition of the system. The metallic state appears with the ferromagnetic state. We have numerically investigated the time evolution of the coupled electronic and spin states by combining the exact diagonalization and the Landau-Lifschitz-Gilbert equation. Due to the effect of the Gilbert dumping, the excited electronic state goes back to the ground state. In the light of the theoretical results, we will discuss the relaxation process and cross-effects in the system with a first-order metal-insulator transition.

10:24AM V29.00013 Chiral spin states in the pyrochlore Heisenberg magnet: Fermionic mean-field theory and variational Monte Carlo calculations, JUNGHOO KIM, JUNG HOON HAN, Sungkyunkwan University — Fermionic mean-field theory and variational Monte Carlo calculations are employed to shed light on the possible uniform ground states of the Heisenberg model on the pyrochlore lattice. Among the various flux configurations, we find the chiral spin states carrying $\pi / 2$ flux through each triangular face to be the most stable both within the mean-field theory and the projected wave- function studies. Properties of the spin-spin correlation function and the chirality order parameter are calculated for the projected wave functions. Meanfield band structures are examined.

10:36AM V29.00014 Spectral properties of orbital polarons in Mott insulators1, KRZYSZTOF WOHLFELD, Jagiellonian University, Cracow, MARIAN DAGHOFER, Oak Ridge National Lab, University of Tennessee, ANDRZEJ M. OLES, Jagiellonian University, Cracow, Max-Planck-Institut FKF, Stuttgart, PETER HORSCH, Max-Planck-Institut FKF, Stuttgart — Since orbital symmetry is lower than SU(2), superexchange in Mott insulators with orbital degrees of freedom is typically not Heisenberg-like and hole propagation is highly nontrivial [1]. We investigate cases with Ising-like superexchange, where the hole cannot propagate by its coupling to spin fluctuations. We find that the usually neglected three-site hopping determines hole motion [2]. One realization of Ising superexchange is the Falicov-Kimball model, where only electrons with one orbital flavor can move, and the other ones are localized — then a hole inserted into the Mott insulator either moves via three-site hopping processes, or remains trapped in a small polaron. In another case of Ising exchange, a class of $t_{2g}$ or $e_g$ orbital systems, renormalized three-site hopping leads to one-dimensional hole propagation, with its direction determined by the orbital flavor of the hole.

1Supported by the Foundation for Polish Science (FNP), the Polish Research Project N202 068 32/1481, and the NSF grant DMR-0706020.
10:48AM V29.00015 Spin conservation and Fermi liquid near a Pomeranchuk transition. ANDREY CHUBUKOV, University of Wisconsin, DMITRII MASLOV, University of Florida — We analyze system behavior near a Pomeranchuk instability in terms of Fermi liquid theory. We argue that the original assumption that a single Landau parameter approaches \(-1\) at a Pomeranchuk transition, while others are non-critical in \(D \leq 3\). We show that, near the transition, a system enters into a novel regime in which all other Landau components increase and eventually diverge at the critical point. We demonstrate that in this novel regime the relation between the Landau function and the full vertex is different from that in a conventional Fermi liquid theory — the proportionality factor 
\[ g \] contains its running effective mass, and has a value near \(-1\) for the boundary between a conventional Fermi liquid and the novel Fermi liquid behavior. We show how to restore spin conservation near a Pomeranchuk transition and discuss extra features specific to Pomeranchuk instabilities in the spin channel.

Thursday, March 19, 2009 8:00AM - 11:00AM – Session V30 DMP GMAG: Focus Session: Multiferroic Properties of Oxide Films

8:00AM V30.00001 Understanding Magnetism in Multiferroics. MIKIEL HOLCOMB, University of California Berkeley — Multiferroics are interesting materials not only because of their exciting order parameters, but for the potential for parameter coupling. In order to understand the magnetoelectric coupling, the individual order parameters must first be understood. BiFeO\(_3\) (BFO), a room temperature ferroelectric and an antiferromagnet, is an excellent model system for understanding the coupling between ferroelectricity and magnetism. A combination of in-plane and out-of-plane piezoelectric microscopy (PFM) allows 3D mapping of the ferroelectric polarization directions in micron-sized regions of the films. The magnetic order of BFO was obtained by using x-ray linear dichroism images using a photoelectron emission microscope (PEEM). When compared with our dichroism models, angle and temperature dependent absorption measurements allow decoupling and direction determination of the two order parameters, ferroelectric and magnetic, contributing to the photoemission signal. These studies reveal a strain-driven reduction in magnetic symmetry in thin films, leading to the formation of a preferred magnetic axis as opposed to the observed easy plane for bulk films. This reduction along with the previous proof of FE-AFM coupling allows electrical control of its magnetic axis. This electrical BFO control has a strong effect on ferromagnets even at room temperature.

8:36AM V30.00002 Infrared and Raman spectroscopy of the magneto-electric coupling in BiFeO\(_3\) films. PETER MAKSYMOWYCH, THOMAS K. LEFIN, Lawrence Berkeley National Laboratory, TN, 73831, SERGEY LESENKO, LAURENT BELLICAHE, University of Arkansas, AK, 72701, NINA BALKE, MARK HUIJBEN, RAMAMOORTHY RAMESH, University of California, Berkeley, CA, 94720, ARTHUR P. ADDARDO, Oak Ridge National Laboratory, TN, 73831, SERGEI V. KALININ, Oak Ridge National Laboratory, TN 73831 — The ferroelectric size effect is a highly pursued and controversial topic encompassing the scaling of polar distortion, domain structure and switchable polarization. We have studied epitaxial BiFeO\(_3\) films using ultrahigh vacuum piezoelectric microscopy and high temperature data, up to 1200 K, on ceramics (infrared) or single crystals (Raman) also show phonon frequency renormalization at the Néel temperature. Our results reinforce a picture where the ferroelectric character of BiFeO\(_3\) plays an important role.

8:48AM V30.00003 Ferroelectric Size-effect on BiFeO\(_3\) Films in Ultra-high Vacuum. PETER MAKSYMOWYCH, STEPHEN JESSE, Oak Ridge National Laboratory, TN, 73831, SERGEY LESENKO, LAURENT BELLICAHE, University of Arkansas, AK, 72701, NINA BALKE, MARK HUIJBEN, RAMAMOORTHY RAMESH, University of California, Berkeley, CA, 94720, ARTHUR P. ADDARDO, Oak Ridge National Laboratory, TN, 73831, SERGEI V. KALININ, Oak Ridge National Laboratory, TN 73831 — The ferroelectric size effect is a highly pursued and controversial topic encompassing the scaling of polar distortion, domain structure and switchable polarization. We have studied epitaxial BiFeO\(_3\) films using ultrahigh vacuum piezoelectric microscopy and high temperature data, up to 1200 K, on ceramics (infrared) or single crystals (Raman) also show phonon frequency renormalization at the Néel temperature. Our results reinforce a picture where the ferroelectric character of BiFeO\(_3\) plays an important role.

9:00AM V30.00004 Electrical conduction at domain walls in multiferroic BiFeO\(_3\). JAN SEIDEL, LANE MARTIN, QING HE, UC Berkeley, QIAN ZHAN, Lawrence Berkeley National Lab, YING-HAO CHU, National Chiao Tung University, Taiwan, AXEL ROTHER, TU Dresden, Germany, MICHAEL HAWKIDGE, Lawrence Berkeley National Lab, PETER MAKSYMOWYCH, Oakridge National Lab, PU YU, MARTIN GAJK, NINA BALKE, UC Berkeley, SERGEI KALININ, Oakridge National Lab, SYBILLE GEMMING, TZ Dresden-Rossendorf, Germany, FENG WANG, UC Berkeley, GUSTAV ATZEL, JAMES SCOTT, Unigemt, and M. JOSEPH ORENSTEIN, RAMAMOORTHY RAMESH, UC Berkeley — We report the observation of room temperature electronic conductivity at ferroelectric domain walls in BiFeO\(_3\). The origin and nature of the observed conductivity is probed using a combination of conductive atomic force microscopy, high resolution transmission electron microscopy and first-principles density functional computations. We show that a structurally driven change in both the electrostatic potential and local electronic structure (i.e., a decrease in band gap) at the domain wall leads to the observed electrical conductivity. We estimate the conductivity in the wall to be several orders of magnitude higher than for the bulk material. Additionally we demonstrate the potential for device applications of such conducting nanoscale features.

9:12AM V30.00005 Ferroelastic domain formation in epitaxial La\(_{0.7}\)Sr\(_{0.3}\)MnO\(_3\) thin films. TIM FISTER, DILLON FONG, JEFFREY EASTMAN, PAUL FUOSS, Materials Science Division, Argonne National Laboratory, KAVAIPTALI BALASUBRAMANIAM, PAUL SALVADOR, Department of Materials Science & Engineering, Carnegie Mellon University — Epitaxial La\(_{0.7}\)Sr\(_{0.3}\)MnO\(_3\) (LSMO) thin films are known to form domains to reduce substrate-induced strain. For instance, on cubic SrTiO\(_3\) (100), LSMO thin films can have up to four rhombohedrally-strained variants. These individual strain states can distort the MnO\(_6\) octahedra and lead to unique electrical and magnetic properties. We have used synchrotron x-ray diffuse scattering to probe the in- and out-of-plane domain structure of a 5 nm LSMO film grown on SrTiO\(_3\) (100). Satellites are present near integer order and half-order peaks. This study exhibits two important points: first, the bounding phase of LSMO domains, and second, the strain state of each variant. Implications of the domain structure on magnetic properties will be discussed.

9:24AM V30.00006 Development of All Oxide Exchange Bias Systems. DAVID KIRKWOOD, Department of Materials and Science and Engineering, University of Virginia, Charlottsville, VA 22904, YONGHANG PEI, Department of Physics, University of Virginia, Charlottesville, VA 22904, NAM DAO, JIWEI LU, STUART WOLF, Department of Materials Science and Engineering, University of Virginia, Charlottsville, VA 22904 — Multiferroic materials exhibit multiple states of order which are often coupled. Bismuth Ferrite (BFO\(_3\)) is a room temperature antiferromagnetic, ferromagnetic materials, where electrical control of magnetism and vice versa has been established. BFO\(_3\) with ferromagnetic oxides such as Magnetite (Fe\(_3\)O\(_4\)) or Lanthanum Strontium Manganite (L\(_2\)S\(_3\)MO\(_3\)) could yield interesting system with electrically controllable exchange bias. We have used a novel deposition tool employing two pulsed electron beam sources (PEBS) to deposit epitaxial layers of BFO\(_3\), LSMO, and Fe\(_3\)O\(_4\) onto STO, LAO, and MgO substrates. We are in the process of making bilayers of these materials and examining the quality and influence of the oxide interface on the development and control of the exchange bias.

1This work is supported by funding from the ARO contract # W911NF-08-2-0032.

2This work is supported by the US DOE, ONR MURI, NSF Chemical Bonding Center program, and the Alexander von Humboldt Foundation.
9:36AM V30.00007 Growth and characterization of multiferroic BiMnO$_3$ thin films$^1$, AMLAN BISWAS, G. SINGH-BHALLA, CHELSEY MORIEN, HYOUNG JEEN JEEN, PATRICK MICKEL, SEFAATIN TONGAY, JULIA NEFF, A. F. HEBARD, Department of Physics, University of Florida, Gainesville, FL 32611 — BiMnO$_3$ is a rare single phase, multiferroic compound which displays both ferromagnetic and ferroelectric properties. However, it is complicated to grow thin films of BiMnO$_3$ due to the volatility of bismuth and substrate induced strain. We have grown thin films of BiMnO$_3$ on SrTiO$_3$ (100) substrates using pulsed laser deposition. These films have a ferromagnetic $T_C$ of about 95 K and electric polarization vs. electric field curves have confirmed their ferroelectric properties. The structure and chemical composition of these thin films have been characterized using x-ray diffraction, atomic force microscopy, scanning electron microscopy, and Auger electron spectroscopy. We will present evidence of the sensitivity of the multiferroic properties of BiMnO$_3$ thin films to the growth conditions and substrate induced strain.

$^1$Supported by NSF DMR-0804452 (AB) and NSF DMR-0704240 (AFH)

9:48AM V30.00008 Multiferroicity in half-doped manganites, SANJEEV KUMAR, Leiden University, GIANLUCA GIOVANNETTI, JEROEN VAN DEN BRINK, SILVIA PICOZZI — Using a joint approach of density functional theory and model calculations, we focus on unconventional physical mechanisms leading to multiferroicity in a prototypical half-doped manganite, La$_{0.5}$Ca$_{0.5}$MnO$_3$. We focus on the strong competition between two exotic charge/orbital-ordered spin ordered states. These are, (1) the charge and orbital ordered zig-zag spin state, also known as the CE-state, and (2) a spin-dimer Zener-polaron state. Both these states respect the inversion symmetry of the lattice and hence can not be ferroelectric. We identify a single variational parameter in terms of the coherent rotation of spin-dimers which interpolates between these two ordered states. It is shown that the true groundstate could be intermediate between these two and can break the inversion symmetry of the lattice. Using DFT calculations we show that the groundstate is indeed ferroelectric with a polarization up to few $\mu C/cm^2$.

10:00AM V30.00009 Element specific magnetic moments of Ni and Mn in multiferroic Bi$_2$NiMnO$_6$ film grown on SrTiO$_3$ substrate , VEMURU KRISHNAMURTHY, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, DAVE KEAVNEY, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, DAVID SINGH, Materials Science and Tech. Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA, A. VENIMADHAV, Department of Cryogenic Engineering, Indian Institute of Technology, Kharagpur 721302, India, Q. LI, Department of Physics, Penn State University, University Park, Pennsylvania 16802, USA — X-ray magnetic circular dichroism (XMCD) and x-ray absorption spectroscopy (XAS) at Ni L$_2$ of Cryogenic Engineering, Indian Institute of Technology, Kharagpur 721302, India, Q. LI, Department of Physics, Penn State University, University Park, Pennsylvania 16802, USA — X-ray magnetic circular dichroism (XMCD) and x-ray absorption spectroscopy (XAS) at Ni L$_2$ and Mn K$_2$ edges have been performed at 4.5 K and higher temperatures in a multiferroic thin film grown on SrTiO$_3$(001) substrate. These spectra show that Ni is in a disordered state and Mn is in a tetrahedral state. The total magnetic moment of Mn is found to be about 2.8 $\mu_B$ at 0.2 K. The total magnetic moment at the Ni site is strongly reduced from the 2.0 $\mu_B$ expected for divalent Ni. We have also detected a small orbital magnetic moment at both Mn and Ni sites. We suggest that the weaker crystal fields at the Ni and Mn sites in the thin film give rise to an orbital moment. These results will be compared with the predictions of local spin density calculations. Supported by US Dept. of Energy.

10:12AM V30.00010 Field Modulated Intrinsic Positive Exchange Bias in Novel Ferrite Ru$_{25}$Cr$_{75}$O$_{77}$ near the Compensation Point , KEVIN G. WEST, NAM DAO, University of Virginia, JIWEI LU, STUART A. WOLF — In some ferrimagnetic materials systems a compensation point is observed where the opposing sublattice magnetizations are equal and opposite resulting in a zero net magnetization. The resulting magnetization decreases below zero at temperatures below $T_C$ and then increase to zero at $T_C$. We observe this type of unusual ferrimagnetic behavior in the Ru$_{25}$Cr$_{75}$O$_{77}$ system. In addition, near the compensation point we observe positive exchange bias that can be modulated using an external applied magnetic field. Possible mechanisms will be discussed.

10:24AM V30.00011 Polarization Coupling in Ferroelectric Multilayers as a Function of Interface Charge Concentration , MAHMUT OKATAN, Institute of Materials Science, University of Connecticut, CT, 06269, JOSEPH MANTESSE, United Technologies Research Center, East Hartford, CT, 06108, PAMIR ALPAY, Institute of Materials Science, University of Connecticut, Connecticut, CT, 06269 — Intriguing properties of multilayered and graded ferroelectrics follow from the electrostatic and electromechanical interactions. The strength of the interlayer coupling depends on the concentration of interfacial defects with short-range local electrostatic fields. Defects may locally relax polarization differences and thus reduce the commensurate bound charge concentration at the interlayer interfaces. In this talk, we develop a theoretical analysis based on non-linear thermodynamics coupled with basic electrostatic relations to understand the role of charge compensation at the interlayer interfaces. The results show multilayered ferroelectrics with systematic variations in the composition may display a colossal dielectric response depending upon the interlayer electrostatic interactions. It is expected that other properties such as the pyroelectric and piezoelectric response will yield concomitant increases through the dielectric permitivity.

The work at UConn was supported by the U.S. Army Research Office through Grant Nos. W911NF-05-1-0528 and W911NF-08-C-0124.

10:36AM V30.00012 Magnetolectric effects in SrRuO$_3$/BaTiO$_3$ heterostructures: A First Principles Study , M.K. NIRANJAN, J.D. BURTON, S.S. JASWAL, E.Y. TSYMBAL, University of Nebraska, Lincoln, USA, J.P. VELEV, University of Puerto Rico, San Juan, USA — Ferroelectric materials in combination with ferromagnets have emerged as structures in which strong magnetoelastic coupling may exist originating from unconventional physical mechanisms. The use of oxides such as SrRuO$_3$ as a metal electrode has been found to be of fundamental importance for the realization of ferroelectric films with critical thicknesses down to three unit cells. Here we present a study of SrRuO$_3$/BaTiO$_3$ heterostructures within the framework of density functional theory. This heterostructure is interesting since SrRuO$_3$ is a weak ferromagnetic oxide metal and hence, when used as an electrode on BaTiO$_3$, presents the possibility of coupling between electric and magnetic order parameters. In particular we study the magnetoelastic (ME) effect at the interface of SrRuO$_3$/BaTiO$_3$ by treating SrRuO$_3$ as spin polarized metal. We find that magnetic properties at the interface are affected as the ferroelectric polarization in the BaTiO$_3$ is reversed. We discuss the origins of ME effect and compare them with previously proposed ME coupling mechanisms in Fe/BaTiO$_3$, Fe$_2$O$_3$/BaTiO$_3$, and SrRuO$_3$/SrTiO$_3$ heterostructures$^{1,2}$. $^1$Niranjjan et al., Phys. Rev. B, 78, 140405 (2008); $^2$Rondinelli et al., Nat. Nanotechnology, 3, 46 (2008).

10:48AM V30.00013 Surface Magnetoelectric Effects from First Principles , CHUN-GANG DUAN, Key Laboratory of Polarized Materials and Devices, East China Normal University, Shanghai, China, CE-WEN NAN, Department of Materials Science and Engineering, Tsinghua University, Beijing, China, SITARAM S. JASWAL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska, USA — A magnetoelastic effect allows magnetic properties of materials by applying electric fields which may be interesting for potential technological applications such as electrically controlled magnetic data storage. We use density functional calculations to reveal and elucidate magnetoelastic effects due to an electric field applied to ferromagnetic metal surfaces. $^1$We find that the surface magnetoelastic effect originates from spin-dependent screening of the electric field and leads to notable changes in the surface magnetization and the surface magnetocrystalline anisotropy. If the ferromagnet is a half-metal the screening charge is formed entirely by a single conducting spin channel which leads to the surface magnetoelastic coefficient being the universal constant $\mu_B/2e^2 \approx 6.44 \times 10^{-14}$ Gcm$^2$/V. This is in an excellent agreement with our first-principles calculation result for the half-metal CrO$_2$. These results are of considerable interest in the area of electrically-controlled magnetism and magnetoelectric phenomena. 1. C.-G. Duan et al., Phys. Rev. Lett. 101, 137201 (2008).
estimate the order parameter to be $M^2$ for a square lattice with an error comparable to quantum Monte Carlo. For the triangular lattice, we verify the existence of three-sublattice magnetic order, and

1 diagram of the frustrated ferromagnetic couplings,

1 Jonas Gustafsson, Goldman Sachs, Daoxin Yao, Erica Carlson, Purdue University, Anders Sandvik, Boston University — We study the system on clusters with a cylindrical geometry to test for the presence of the order.

3 Queensland, Dept of Physics — We show that dimer coverings on the star lattice (aka the 3-12, Fisher, expanded kagome or triangle-honeycomb lattice) have

L $\sim$ Combining the improved DMRG accuracy with the use of non-traditional clusters for rapidly converging finite-size scaling, we study the ordering in the square-

1 aspect ratio depends on the boundary conditions, with a simple and convenient choice being precisely the geometry optimal for the DMRG method. Combining the improved DMRG accuracy with the use of non-traditional clusters for rapidly converging finite-size scaling, we study the ordering in the square-

1 aspect ratio ($l_x/l_y$ close to 2), in agreement with the effective $\sigma$-model. We determine the thermodynamic limit of $M$ for the square lattice with an error comparable to quantum Monte Carlo. For the triangular lattice, we verify the existence of three-sublattice magnetic order, and estimate the order parameter to be $M = 0.205(15)$.

1 Supported by the DOE (DE-FG02-04ER46174, S.C.) and NSF (DMR-0605444, S.W.)

8:24AM V31.00003 Classical and quantum dimers on the star lattice

1 John Fjaerestad, University of Queensland, Dept of Physics — We show that dimer coverings on the star lattice (aka the 3-12, Fisher, expanded kagome or triangle-honeycomb lattice) have $Z_2$ arrow and pseudo-spin representations analogous to those for the kagome lattice, and use these to construct an exactly solvable quantum dimer model (QDM) with a Rokhsar-Kivelson (RK) ground state. This QDM, first discussed by Moessner and Sondhi from a different point of view, is the star-lattice analogue of a kagome-lattice QDM analyzed by Misguich et al. We discuss various properties of the classical equal-weight dimer model on the star lattice, most of which are related to those of the RK state. Using both the arrow representation and the fermionic path integral formulation of the Pfaffian method, we calculate the number of dimer coverings, dimer occupation probabilities, and dimer, vison, and monomer correlation functions. The results show unusual features similar to those of dimers on the kagome lattice. We also discuss some generalizations to general Fisher lattices and their “reduced” lattices (the kagome, squagome, and triangular-kagome lattice being examples of the latter). Ref.: J. O. Fjaerestad, arXiv:0811.3789

1 Research supported by the Australian Research Council

8:36AM V31.00004 Spatially anisotropic Heisenberg kagome antiferromagnet

, Oleg Starykh, University of Utah — We study the quasi-one-dimensional limit of the spin-1/2 quantum Heisenberg antiferromagnet on the kagome lattice. The lattice is divided into antiferromagnetic spin-chains (exchange $J$) that are weakly coupled via intermediate “dangling” spins (exchange $J'$. Using one-dimensional bosonization, renormalization group methods, and current algebra techniques the ground state is determined in the limit $J' \ll J$. We find that the dangling spins and chain spins form a spiral with $O(1)$ and $O(J'/J)$ static moments, respectively, atop of which the chain spins exhibit a smaller $O((J'/J)^2)$ antiferromagnetically ordered component along the axis perpendicular to the spiral plane. We describe similarities and differences of our findings with other recent studies, based on semi-classical and large-N approaches. Critical comparison of quasi-one-dimensional kagome antiferromagnet with other quasi-one-dimensional models will be presented as well.

9:12AM V31.00005 Ordered States on the Kagome Antiferromagnetic Heisenberg Model

, Simeng Yan, Steven White, University of California, Irvine — We numerically study the spin 1/2 Kagome antiferromagnetic Heisenberg Model with DMRG techniques. Recently, Singh and Huse proposed a dimerized ground state with a 36 site unit cell. To test this proposal, we have simulated the system on clusters which favor this order. If the order was not found, this would disprove the proposal. However, the results do show the proposed order. The strength of the dimerization on the pinwheels is surprisingly strong, with $<S \cdot S>$ taking values of -0.71 on the strong bonds and -0.11 on the weak. We also have studied the system on clusters with a cylindrical geometry to test for the presence of the order.

9:24AM V31.00006 Universality Classes of Dimerized Bond-Disordered Quantum Spin Models

, Jonas Gustafsson, Goldman Sachs, Daoxin Yao, Erica Carlson, Purdue University, Anders Sandvik, Boston University — We study the dimerized bond disordered $S=1/2$ Heisenberg models on the square lattice. Each spin belongs to one strong bond (a dimer) by introducing strong and weak couplings, $J_x, J_y$. By means of quantum Monte Carlo simulations, we find two different universality classes for the random dimer model and the random plaquette model. The change of universality class may be associated with the cancellation of Berry phase. Furthermore, we study the dilution effect by setting some strong bonds to 0.

9:36AM V31.00007 Emergent multipolar spin correlations in a fluctuating spiral - The frustrated ferromagnetic $S=1/2$ Heisenberg chain in a magnetic field

, Andreas Lauchli, Max Planck Institute for Physics of Complex Systems, Dresden, Germany, Julien Sudan, Andreas Luscher, IRMA - EPF Lausanne, Switzerland — We present the phase diagram of the frustrated ferromagnetic $S=1/2$ Heisenberg $J_x,J_y$ chain in a magnetic field, obtained by large scale exact diagonalizations and density matrix renormalization group simulations. A vector chirally ordered state, metamagnetic behavior and a sequence of spin-multipolar Luttinger liquid phases up to hexadecapolar kind are found. We provide numerical evidence for a novel locking mechanism, which can drive spiral states towards spin-multipolar phases, such as quadrupolar or octupolar phases. Our results also shed new light on previously discovered spin-multipolar phases in two-dimensional $S=1/2$ quantum magnets in a magnetic field. We conclude by presenting numerical results on the dynamical spin structure factor in the various phases which are valuable in identifying multipolar phases in experiments.
Dynamically dominant excitations of string solutions in the antiferromagnetic Heisenberg chain in magnetic fields. MASANORI KOHNO, International Center for Materials Nanoarchitectonics, NIMS — We investigate behaviors of dynamical structure factors in the spin-1/2 antiferromagnetic Heisenberg chain in magnetic fields, using Bethe-ansatz solutions. We uncover a well-defined continuum in $S^{z}(k,\omega)$, which comes from 2-string solutions in the Bethe ansatz. It continuously connects the des Cloizeaux-Pearson mode in the zero-field limit and the bound state of overturned spins from the ferromagnetic state near the saturation field. Also, we give a natural interpretation to particles in magnetic fields, psion and antipsion, as those carrying fractional quantum numbers $S^{z}=+1/2$ and $-1/2$, respectively. We argue that not only psions and antipsions but also particles representing strings play important roles for dynamical properties of the antiferromagnetic Heisenberg chain in magnetic fields. We confirm the relevance of the present results to real materials through comparisons with experimental results.

10:00AM V31.00009 Interplay between interaction and (un)correlated disorder in Heisenberg spin-1/2 chains. FRIEDA DUKESZ, MARINA ZILBERGERTS, LEA SANTOS, Yeshiva University — We consider a Heisenberg spin-1/2 chain and study the interplay between the Ising interaction and on-site disorder, while keeping the hopping amplitude constant. Disorder is characterized by both: uncorrelated and long-range correlated random on-site energies. The level of delocalization, quantified by the number of principal components, is largest in clean systems with non-interacting particles. However, in the presence of uncorrelated disorder, delocalization becomes maximum for a non-zero value of the interaction amplitude. The inclusion of long-range correlated disorder may further extend two-particle states, but the effect decreases with the number of excitations and the strength of the interaction, and may even be reversed, as shown for half-filled chains. Quantum correlations, determined by a global entanglement measure, present similar behavior, but the largest value appears for clean systems with interacting particles.

10:12AM V31.00010 Algebraic spin liquid in an exactly solvable spin model. HONG YAO, SHOU-CHENG ZHANG, STEVEN KIVELSON, Stanford University — We have introduced an exactly solvable quantum spin-3/2 model on the square lattice. Its ground state is a spin liquid with half integer spin per unit cell. The fermionic excitations are gapless with a linear dispersion, while the topological “vison” excitations are gapped. Moreover, the massless Dirac fermions are stable against any small perturbations with time-reversal symmetry. Thus, this model is, to the best of our knowledge, the first exactly solvable model whose ground state is an “algebraic spin liquid” with half integer spin per unit cell.

10:24AM V31.00011 Extended supersolid phase of frustrated hard-core bosons on a triangular lattice. FA WANG, FRANK POLLMANN, ASHVIN VISHWANATH, UC Berkeley — We study a model of hard-core bosons with frustrated nearest-neighbor hopping (t) and repulsion (V) on the triangular lattice. We argue for a supersolid ground state in the large repulsion limit (V >> |t|) limit where a dimer representation appears. By constructing a unitary mapping to the well understood unfrustrated hopping case, this generalized ‘Marshall sign rule’ allows us to establish the precise nature of the supersolid order by utilizing a recently proposed dimer variational wavefunction, whose correlations can be efficiently calculated using the Grassmann approach. By continuity, a supersolid is predicted over the wide parameter range, V -2|t| > 0. This also establishes a simple phase diagram for the triangular lattice spin 1/2 XXZ antiferromagnet.

10:36AM V31.00012 A Γ-matrix generalization of the Kitaev model. HSING-HSUAN HUNG, CONGJUN WU, DANIEL AROVAS, University of California, San Diego — We extend the Kitaev model defined for the Pauli-matrices to the Clifford algebra Γ-matrices by taking the 4x4 representation as an example. In a 2D decorated square lattice, the ground state spontaneously breaks time-reversal symmetry and exhibits a topological phase transition. The topologically non-trivial phase carries gapless chiral edge modes along the sample boundary. In the 3D diamond lattice, the ground states exhibit gapless 3D Dirac cone-like excitations and gapped topological insulating states. The generalizations to even higher rank Γ-matrices are also discussed.

10:48AM V31.00013 Dzyaloshinskii-Moriya interactions in valence bond systems II. MAYRA TOVAR, KUMAR RAMAN, KIRILL SHTENGEL, UC Riverside — We investigate the effect of Dzyaloshinskii-Moriya interactions on the low temperature magnetic susceptibility for a system whose low energy physics is dominated by short-range valence bonds (singlets). Our general perturbative approach is applied to specific models expected to be in this class, including the Shastry-Sutherland model of the spin-dimer compound SrCu$_2$(BO$_3$)$_2$ and the antiferromagnetic Heisenberg model of the recently discovered $S = 1/2$ kagome compound ZnCu$_3$(OH)$_6$Cl$_2$. The central result is that a short-ranged valence bond phase, when perturbed with Dzyaloshinskii-Moriya interactions, will remain time-reversal symmetric in the absence of a magnetic field but the susceptibility will be nonzero in the zero temperature limit. Applied to ZnCu$_3$(OH)$_6$Cl$_2$, this model provides an avenue for reconciling experimental results, such as the lack of magnetic order and lack of any sign of a spin gap, with known theoretical facts about the kagome Heisenberg antiferromagnet.

— NSF DMR-0749295

Thursday, March 19, 2009 8:00AM - 10:24AM — Session V32 GMAG DMP FIAP: Focus Session: Vortex and Domain Wall Dynamics 336

8:00AM V32.00001 Dynamics of Exchange-Biased Magnetic Vortices. T. Y. CHEN, M. K. CHAN, P. A. CROWELL, University of Minnesota — We have studied magnetization dynamics in micron-sized circular disks composed of ferromagnetic (FM)-antiferromagnetic (AFM) bilayers. The patterned samples of FeMn/NiFe are field-cooled (FC) or zero-field cooled (ZFC) from above the blocking temperature to room temperature. Time-resolved Kerr microscopy measurements show that the vortex gyrotropic mode fluctuates in frequency as the vortex core is displaced by a static in-plane magnetic field. The average gyrotropic frequency and the magnitude of its fluctuations, which are due to pinning of the vortex core, are larger than in single layer films. The enhancement of the gyrotropic frequency is largest in the ZFC samples, in which the effective field due to exchange coupling is expected to enhance pinning of the vortex core at the center of the disk. We find, however, that micromagnetic simulations incorporating uniform or vortex-like exchange-bias fields do not explain our results quantitatively. We interpret this discrepancy as a consequence of randomly oriented AFM domains, which are comparable in size to the vortex core. This work was supported by NSF and the Univ. of Minnesota Graduate School.

8:12AM V32.00002 Ferromagnetic resonance force spectroscopy of a magnetic vortex. G. DE LOUBIES, J. O. KLEIN, N. SPEC, CEA Saclay, A. RIEGLER, F. LOCHNER, G. SCHMIDT, L.W. MOLENKAMP, Universität Würzburg, H. HURDEQUINT, LPS, Orsay, F. BOUST, ONERA, N. VUKADINOVIC, Dassault Aviation, A.N. SLAVIN, Oakland University — Due to its nanometer size (of the order the exchange length), probing the high frequency dynamics of a magnetic vortex core is an experimental challenge. Precessional dynamics of the magnetization of individual nano-disks of NiMnSb perpendicularly magnetized is measured in a wide range of bias magnetic fields using a magnetic resonance force microscope (MRFM). A full dynamic phase diagram, demonstrating excitation of a Kittel-type dipolar mode in the saturated disks and the gyrotropic mode of vortex core rotation in the vortex-state unsaturated disks, is established. Switching of the vortex core polarity in a negative (anti-parallel to core) bias magnetic field is registered dynamically. Analytic theory and micromagnetic simulations provide a quantitative description of the experimental results.
8:24AM V32.00003 Spin motive electric field driven by magnetic vortex motion. JUN-ICHIRO OHE, Tohoku University, STEWART E. BARNES, University of Miami, SADAMICHI MAEKAWA, Tohoku University — The current-induced magnetization dynamics realized in spintronics devices involve both of charge and spin degrees of freedom. Recently, it has been pointed out that the magnetization dynamics induces an effective electric field acting on the conduction electrons through the spin Berry phase. The effective electric field, or a “spin motive electric field,” was investigated for a simple one-dimensional domain wall. It is difficult to estimate analytically this effective electric field in actual systems, because the magnetization dynamics obeys the non-linear Landau-Lifshitz equation. In this report, we describe numerical studies of the spin motive electric field induced by the dynamics of a vortex core. The vortex structure can be realized in a Permalloy disc. It is known that the magnetic vortex core shows a resonant motion when the oscillating magnetic field is applied. The direction of the core is switched rapidly by applying a pulsed such magnetic field. During the core motion, we obtain an electric field near the core. The direction of the electric field is perpendicular to the direction of the core motion. We also obtain the electric field driven by spin waves which are excited by the core switching. We propose an experimental setup for measuring the electric field. The calculated voltage is large enough to measure. We show that the voltage induced by core switching is quite large.

8:36AM V32.00004 Thickness and field dependence of the driven dynamic mode-splitting of magnetic vortices1, KRISTEN BUCHANAN, Colorado State University — We have explored the effects of increased driving field amplitude on the dynamics of magnetic vortices using a microwave reflection technique and found that the vortex translational eigenmode profile first takes on a distorted shape and then splits into two well-defined peaks as the field is increased [1]. Here we examine the thickness and field dependence of this mode-splitting phenomenon via measurements of lithographically patterned micron-sized Permalloy ellipses with thicknesses of 20, 40, and 60 nm. The experimental results will be compared to numerical calculations that incorporate a critical velocity parameter and provide new insight into the origin of the observed vortex dynamic mode splitting. Acknowledgments: Thank you to Marcos Grimsditch, Frank Fradin, Sam Bader, and Val Novosad for stimulating discussions. [1] Buchanan et al. PRL 99,267201 (2007).


9:00AM V32.00006 High frequency spin dynamics in soft magnetic dots in biased vortex state: precise probing and nature of the eigenmodes1, FARKHAD ALIEV, JUAN FRANCISCO SIERRA, AHMAD AWAD, Universidad Autonoma de Madrid, GLEB KAKAZEI, Universidade do Porto, DONG-SOO HAN, Seoul National University, SANG-KOONG KIM, HONGKI MIN, TOHOKU UNIVERSITY, KRISTEN BUCHANAN, Colorado State University — We have explored the effects of increased driving field amplitude on the dynamics of magnetic vortices using a microwave reflection technique and found that the vortex translational eigenmode profile first takes on a distorted shape and then splits into two well-defined peaks as the field is increased [1]. Here we examine the thickness and field dependence of this mode-splitting phenomenon via measurements of lithographically patterned micron-sized Permalloy ellipses with thicknesses of 20, 40, and 60 nm. The experimental results will be compared to numerical calculations that incorporate a critical velocity parameter and provide new insight into the origin of the observed vortex dynamic mode splitting. Acknowledgments: Thank you to Marcos Grimsditch, Frank Fradin, Sam Bader, and Val Novosad for stimulating discussions. [1] Buchanan et al. PRL 99,267201 (2007).

9:12AM V32.00007 Spin-Torque Ferromagnetic Resonance Spectroscopy of Permalloy Nanowires, CARL BOONE, JORDAN KATINE, JEFF CHILDRESS, JIAN ZHU, XIAO CHENG, ILYA KRIVOROTOV, KRIVOROTOV GROUP COLLABORATION, HITACHI GLOBAL STORAGE COLLABORATION — We develop a technique for studies of spectral properties of spin waves excited by spin transfer torque in metallic ferromagnetic nanowires, and apply this technique to measure frequencies and damping constants of several low-energy quantized spin wave modes in permalloy nanowires of rectangular cross section. Our measurements demonstrate that the spin wave spectrum of nanowires as narrow as 100 nm is well described by an analytic theory of dipole-exchange spin waves in thin ferromagnetic strips. Geometric quantization of the spin wave spectrum in nanowires significantly reduces the phase space for magnon-magnon scattering leading to opening and closing of discrete scattering channels as a function of magnetic field. These scattering channels manifest themselves as peaks in plots of spin wave damping versus magnetic field. In particular, we observe damping enhancement of the lowest energy spin wave mode at the values of magnetic field corresponding to three-magnon confluence processes in which two lowest energy magnons merge into a single higher-energy mode magnon.

9:24AM V32.00008 Effects of disorder and temperature on vortex domain wall dynamics1, HONGKI MIN, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899-6202, MICHAEL DONAHUE, Mathematical and Computational Sciences Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8910, MARK STILES, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899-6202 — Domain wall motion, whether driven by applied magnetic fields or electrical current, can be strongly affected by sample irregularities. Using micromagnetic simulations and a collective coordinate approach, we study the dynamics of domain wall motion driven by a spin-polarized current or an external magnetic field in the presence of extrinsic random potential at finite temperatures. We compare these calculations and discuss the region of validity of the approximations in the simple model. Information about the strength of the random potential is taken from recent magnetic resonance experiments.

1This work was supported by Colorado State University and by DOE contract number DE-AC02-06CH11357.
2The work was supported by Spanish MEC (MAT2006-07196) and by Creative Research Initiatives of MOST/KOSEF
3This work has been supported in part by the NIST-CNST/UMD-NanoCenter Cooperative Agreement.
on a DW in terms of an electron drift speed \( u = -\frac{P*J}{\mu_B} \) where \( \mu_B \) is the Bohr magneton and \( M \) the saturation magnetization. While appropriate for adiabatic torques, this quantity \( u \) is misleading and not the best choice in the case of non-adiabatic torques. For example, it leads to beta not equal to alpha, where beta represents the intensity of the non-adiabatic torque, and alpha is the damping parameter. By writing equations of motion for conduction- electron spins in a moving frame where the electron gas is at rest, we find a direct relation between damping and non-adiabatic torques. The correct electron drift speed turns out to be the speed of the frame, and is \( v = \frac{P*J}{(n*q)} \) where \( n \) and \( q \) are the carrier density and charge. It is related to the ordinary Hall constant \( R_h \) by \( v = \frac{P*R_h}{J} \). After substituting \( v \) for \( u \) in the expression of the non-adiabatic torque, we find that beta = alpha holds now. Because \( v \) is larger than \( u \) in Permalloy, it can explain better the large current-induced DW speeds found \(^4\) experimentally. In materials where \( R_h > 0 \) and the carriers are dominantly hole-like, \( v \) and \( u \) have opposite signs, leading to different predictions for the sense of DW motion. We discuss examples of such materials. \(^1\) G. Tataru and H. Kohno, Phys. Rev. Lett. 92, 086601 (2004). \(^2\) H. Kohno et al., J. Phys. Soc. Japan, 75, 113706 (2006). \(^3\) L. Berger, Phys. Rev. B 75, 174401 (2007).

This work was supported by NSF, DOE and Welch Foundation.
8:24AM V33.00003 Frequency dependence of the intrinsic Hall conductivity in a chiral $p + ip$ superconductor with impurities$^1$. PAVEL NAGORNYKH, ROMAN LUTCHYN, VICTOR YAKOYENKO, University of Maryland — We calculate frequency dependence of the intrinsic Hall conductivity induced by impurity scattering in a chiral $p_x + ip_y$ superconductor. We find that, at large frequencies compared to the superconducting gap ($\Omega \gg \Delta$), the real part of the intrinsic Hall conductivity at zero temperature is proportional to $\Delta/\Omega^3 \log(\Omega/2\Delta)$. Using our results for the Hall conductivity, we estimate the Kerr angle and compare it with the experimental data on Sr$_2$RuO$_4$ by Xia et al., Phys. Rev. Lett. 97, 167002 (2006).

$^1$This work was supported by JQI

8:36AM V33.00004 Electromagnetic response of time reversal invariant triplet superconductors . RAHUL ROY, CATHERINE KALLIN, JOHN BERLINSKY, McMaster University — We study the effective action of time reversal invariant triplet superconductors in two and three dimensions and obtain the electromagnetic response. The B-phase of Helium 3 and its two dimensional analog are topologically non-trivial phases. The two dimensional triplet superconductor may be regarded as two copies of a chiral $p_x + ip_y$ superconductor. We discuss signatures of the non-trivial topology in the effective action and in the electromagnetic response.

8:48AM V33.00005 Microscopic analysis of the stability of half-quantum vortices in $p_x + ip_y$ superfluids in an annular geometry.$^1$. VICTOR VAKARYUK, University of Illinois at Urbana-Champaign — We present a microscopic analysis of the thermodynamic stability of a half-quantum vortex (HQV) in $p_x + ip_y$ variant of equal-spin-pairing state which, under suitable conditions, is believed to be realized in Sr$_2$RuO$_4$ and $^3$He-A. Our approach is based on a description of the HQV in terms of a BCS-like wave function with a spin-dependent boost. Stability criteria are found by comparing energies of half- and full-quantum vortices with appropriate account taken of Fermi liquid corrections. While we confirm earlier phenomenological findings by Suk Bum Chung et al. (2007) for the stability of the HQV in the annular geometry, we also predict a novel feature that the HQV, if exists, should be accompanied by a non-zero spin polarization of the system.

$^1$Supported by the National Science Foundation (DMR03-50842).

9:00AM V33.00006 Josephson tunneling studies of odd-parity superconductivity in Sr$_2$RuO$_4$ , RONALD MYERS, YING LIU, Pennsylvania State University, D. FOBES, Z. MAO, Tulane University, H. YAGUCHI, Y. MAENO, Kyoto University — In the recent phase-sensitive work that provided the most unambiguous evidence for odd-parity superconductivity in Sr$_2$, RONALD MYERS, YING LIU, Pennsylvania State University, D. FOBES, Z. MAO, Tulane University, H. YAGUCHI, Y. MAENO, Kyoto University — In the recent phase-sensitive work that provided the most unambiguous evidence for odd-parity superconductivity in Sr$_2$RuO$_4$, we used Au$_{3,5}$In$_{0,5}$ as the s-wave superconducting counter electrode in the SQUID structure. However, Au$_{3,5}$In$_{0,5}$ has a $T_c$ less than that of Sr$_2$RuO$_4$, making detection of the pairing symmetry near the $T_c$ of Sr$_2$RuO$_4$ inaccessible to the phase sensitive measurements. To go beyond this limit and open up possibilities of several other experiments involving Josephson tunneling into Sr$_2$RuO$_4$, we seek an alternative material system with an s-wave superconductor of $T_c > 1.5K$ that would exhibit Josephson coupling with Sr$_2$RuO$_4$. An Ag/Pb/Pb trilayer has been chosen for this purpose. Ag/Pb/Sr$_2$RuO$_4$ tunneling devices were prepared that showed a suppressed superconducting gap feature of Sr$_2$RuO$_4$, suggesting the presence of superconductivity at the polished ac face of a Sr$_2$RuO$_4$ crystal. However, no Josephson coupling between Ag/Pb and Sr$_2$RuO$_4$ was detected. More experiments are currently underway, and new results will be presented.

9:12AM V33.00007 Measurements of superconducting energy gap in individual Ru islands embedded in Sr$_2$RuO$_4$ , YIQUN YING, B. CLOUSER, R. MYERS, N. STALEY, YING LIU, Pennsylvania State University, D. FOBES, Z. MAO, Tulane University, Y. XIN, Florida State University, J. ALLARD, Oak Ridge National Laboratory — We report our tunneling measurements on individual single-crystalline Ru islands embedded in a bulk Sr$_2$RuO$_4$ single crystal. Tunneling junctions were prepared on large (micron size) and small (submicron size) Ru islands by fabricating tunneling windows using quartz filaments as shadow masks. Our measurements revealed the presence of an energy gap below a temperature close to the $T_c$ of bulk Ru. In the zero temperature limit, the gap was found to be 0.07 meV for large Ru islands, consistent with our measurements on bulk polycrystalline Ru. However, in small Ru islands a gap of 0.1 meV, clearly larger than that seen in large Ru islands, was observed. The difference in energy gap may reflect difference in pairing state in Ru islands of different sizes. Above the $T_c$ of Ru but below the $T_c$ of Sr$_2$RuO$_4$, we detected no proximity induced energy gap. This observation is unexpected as our $^3$He-contrasted transmission electron microscope study showed that the interface between a Ru island and Sr$_2$RuO$_4$ is atomically sharp, which appears to rule out the suppression of the proximity effect by disorder. We argue that these observations are associated with chiral p-wave superconductivity in Sr$_2$RuO$_4$.

9:24AM V33.00008 Magnetic response of Sr$_2$RuO$_4$ nanocrystals: search for chiral currents and fractional vortices$^1$. D. J. BAHR, M. J. A. STOUTIMORE, R. BUDAKIAN, D. J. VAN HARLINGEN, University of Illinois at Urbana-Champaign, Urbana IL, Y. MAENO, Kyoto University, Kyoto, Japan — The ruthenate superconductor Sr$_2$RuO$_4$ may have a chiral order parameter of the form $p_x \pm ip_y$, making it a candidate for nucleation of excitations with non-Abelian statistics that could enable topologically protected quantum computing. To test this scenario, we have measured the magnetic response of Sr$_2$RuO$_4$ nanocrystals to search for spontaneous chiral currents and half-integer vortices. Each nanocrystal ($1 \mu m \times 1.5 \mu m \times 0.5 \mu m$) was extracted from a large single crystal with bulk transition temperature in the range 1.2K-1.4K. We then glued it into the pickup loop of a flux transformer or a gradiometer that is inductively coupled to a dc-SQUID magnetometer. We have observed the diamagnetic screening of the crystal and the entry of discrete vortices in an applied magnetic field. We report on our search for spontaneously generated currents, chiral domain dynamics and the nucleation of half-integer vortices, which we should be sensitive to due to the small size of the crystal.

$^1$Work supported by DOE BES grant DEFG02-07ER46453.

9:36AM V33.00009 Investigating magnetic order in Sr$_2$RuO$_4$ using cantilever torque magnetometry$^1$. RAFFI BUDAKIAN, JOONHO JANG, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, YOSHI MAENO, Kyoto University — Following the initial $^3$He and NMR studies suggesting that Sr$_2$RuO$_4$ is a spin-triplet superconductor, there has been a great deal of interest to understand the nature of the order parameter. Although Sr$_2$RuO$_4$ is similar in structure to the layered high-Tc cuprate superconductors, it is thought to possess chiral $p_x \pm ip_y$ pairing symmetry. The complex order parameter can give rise to a rich variety of new correlated states, such as domains having orbital order that possess a net magnetic moment and half-integer vortices with zero-energy modes. We have applied ultrasensitive cantilever torque magnetometry to measure the magnetic moment, susceptibility, and vortex entry into micron-size Sr$_2$RuO$_4$ in search of magnetic moments generated by chiral edge currents and fractional vortices. This talk will present recent data in this effort.

$^1$Work supported by DOE BES grant DEFG02-07ER46453.
9:48AM V33.00010 Orbital magnetic moment in the chiral p-wave superconductor Sr2RuO4. 
JAMES ANNETT, University of Bristol, KAROL WYSÓKINSKI, M. Curie Skłodowska University, BALÁZS GYORFFY, University of Bristol — The existence and magnitude of a bulk orbital angular momentum of the condensate chiral a phase in superfluid helium-3 is a longstanding matter of controversy. The analogous problem in a chiral p-wave superconducting material is the existence of a finite orbital magnetic moment in the bulk. In Sr2RuO4 the existence of such an orbital moment is strongly suggested by experimental evidence for spontaneously time reversal symmetry breaking (TRS) in the superconducting state, but the theories disagree on the exact magnitude of this moment. We show that a non-zero orbital magnetization density arises naturally in a realistic band model for Sr2RuO4, and its temperature dependence is qualitatively similar to those of the muSr and Kerr effect experimental results. The simplest model which leads to the orbital moment requires at minimum two degenerate atomic orbitals per Ru, which correspond to the Ru d xz and d yz states. This is in contrast to the theories of orbital angular momentum in the isotropic superfluid 3-He, or models of orbital moment in Sr2RuO4 which assume only a single band at the Fermi level. The implications of this surprising result are explored.

10:00AM V33.00011 Absence of superconductivity in the half-filled anisotropic triangular lattice Hubbard model. 
HONGTAO LI, University of Arizona, R.T. CLAY, Mississippi State University, S. MAZUMDAR, University of Arizona — The superconducting κ-(BEDT-TTF)2X salts, with one hole per molecular site and strong dimerization are widely thought to have an effective 1/2-filled band. The presence of antiferromagnetism (AFM) near superconductivity (SC) in their pressure-temperature phase diagram has led to the suggestion suggest that the SC can be explained within an anisotropic triangular lattice 1/2-filled band Hubbard Hamiltonian. In this model increasing frustration suppresses the AFM transition, and it has been suggested that d-wave SC appears near the metal/AFM interface. We performed exact diagonalizations on a 16-site periodic anisotropic triangular lattice and determined the full phase diagram. We confirm the Mott metal-insulator transition and AFM, change of the AFM wavevector for large anisotropy, and the presence of a non-magnetic insulating phase. We do not find any hint of long range superconducting correlations. In our results the Hubbard U always suppresses the superconducting pair-pair correlations over their non-interacting value. We conclude that the Hubbard model is too simple to explain the SC in organic charge-transfer solids.

1Supported by DOE grant DE-FG02-06ER46315.

10:12AM V33.00012 Nuclear spin-lattice relaxation rate as a link between antiferromagnetism and superconductivity in organic conductors. 
CLAUDE BOURBONNAIS, Departement de Physique, Universite de Sherbrooke, Sherbrooke, (QC), Canada J1K-2R1, ABDELOUAHAB SEDEKI, Departement de Physique, Universitede Sherbrooke, Sherbrooke, (QC), Canada J1K-2R1 — The interdependence of antiferromagnetism and superconductivity in the Bechgaard salts series of organic conductors is examined in the light of the anomalous temperature dependence of the nuclear spin-lattice relaxation rate. We use the renormalization group approach to the electron gas model to demonstrate that the metallic state anomaly of the nuclear relaxation rate found in the Bechgaard salts and the mechanism of passage from antiferromagnetism to superconductivity can be both described within a unified framework.

1Supported by National Sciences and Engineering Research Council of Canada (NSERC) and Canadian Institute for Advanced Research (CIFAR).

10:24AM V33.00013 New details in the phase diagram of λ-(BETS)2GaCl4 made by advancing the art of RF penetration depth measurements in pulsed fields using a tunnel diode oscillator. 
WILLIAM A. CONIGLIO, LAUREL E. WINTER, KYUIL CHO, BRAUEN E. SMITH, C.C. AGOSTA, Clark University, L.K. MONTGOMERY, Indiana University — We report improvements to the Tunnel Diode Oscillator method of measuring the penetration depth of a superconductor at RF frequencies above 100 MHz. Optimizations to the circuit for high frequency and pulsed fields are briefly discussed as well as a digital demodulation technique for rendering the oscillation frequency with accuracy suitably better than the stability of the oscillator itself. Using a 390 MHz oscillator, we measured the penetration depth of λ-(BETS)2GaCl4 with the magnetic field oriented parallel to the conducting planes of the sample using fields up to 21 T and temperatures from 400 mK to 5.5K. Our new data crunching techniques have allowed us to resolve two phase transitions between the superconducting and normal states as well as a third transition that appears at low temperature as an enhancement to the upper critical field. We explore the properties of the phase diagram in two samples.

1We acknowledge DOE support from DE-FG02-05ER46214.

LAUREL E. WINTER, WILLIAM A. CONIGLIO, KYUIL CHO, BRAUEN E. SMITH, C.C. AGOSTA, Clark University, L.K. MONTGOMERY, Indiana University — The upper critical fields for the highly anisotropic organic superconductor λ-(BETS)2GaCl4 have been studied by measuring the in-plane RF penetration depth with a tunnel diode oscillator technique in pulsed fields. At zero field we found a Tc of 5 K. With the field perpendicular to the conducting layers we extrapolate Hc2,Τ=0 to 2.8 T and with the field parallel Hc2,Τ=0 is 11 T. With the field applied parallel to the conducting layers, for Τ > 0.5Tc the Hc2 follows the superconducting gap function √1 - Tc/Τ, then saturates below 0.5Tc. Below 0.35Tc we see a clear enhancement of 1.5 T in Hc2 and in addition there is a second phase line at a lower field than Hc2. These features are both characteristic of the FFLO state. We will discuss this second phase line in relation to the Pauli Limit as calculated in a similar empirical method and compare our phase diagram to previous results.

1We acknowledge DOE support from DE-FG02-05ER46214.

10:48AM V33.00015 Mesoscopic conductance oscillations in superconducting nanoparticle films. 
AL-AMIN DHIRANI, BRIAN LAM — Recent advances in nanoparticle synthesis yield control over key nanoparticle characteristics such as structure and chemical composition. This in turn enables fabrication of nanostructured materials with novel and controlled properties. We have found that superconducting 100 nm niobium nanoparticles can be sintered to make porous macroscopic films that routinely exhibit conductance oscillations as a function of bias voltage and magnetic field. We speculate the effect is related to electron-hole interference previously observed at interfaces between disordered normal materials and superconductor electrodes. Our results show that the oscillations in the present system are associated with nanoparticle state (superconducting vs. normal) and ubiquitous elastic scattering at length scales dictated by nanoparticle size. Robust observation of this mesoscopic interference phenomenon in a disordered, macroscopic system is remarkable. It is enabled by the present approach’s ability to balance counterrevering considerations: sufficient disorder to induce elastic scattering and restricted averaging to limit dephasing.

Thursday, March 19, 2009 8:00AM - 11:00AM —
Session V34 DCMP: Superconductivity: Spectroscopy 404
8:00AM V34.00001 Comparing the three characteristic electronic excitations in the pseudogap state of underdoped $\text{Bi}_2\text{Sr}_2\text{Ca}_0.8\text{Y}_{0.2}\text{Cu}_2\text{O}_8$ \cite{1}. K. FUJITA, JHINHWAN LEE, C. K. KIM, A. SCHMIDT, Cornell University, H. EISAKI, NI-AIST Tsukuba, S. UCHIDA, University of Tokyo, J. C. DAVIS, Cornell University and Brookhaven National Laboratory — We investigate the quasiparticle interference processes as a function of temperature for heavily underdoped $\text{Bi}_2\text{Sr}_2\text{Ca}_0.8\text{Y}_{0.2}\text{Cu}_2\text{O}_8$ ($T_c$=42K). We demonstrate that three types of electron excitations exist in the pseudogap phase: (1) metallic excitations on the Fermi Arc, (2) the Bogoliubov quasiparticle excitations of what appears to be a phase incoherent d-wave superconductor in the confined area in momentum space (Jhinwan Lee et al (2009)) and (3) the high energy pseudogap excitations seen in the anti-nodal region outside the $\sqrt{2}x/2$ Brillouin zone (Y. Kohsaka et al. Nature 454, 1072 (2008)). We discuss the relationship of these three components of the electronic structure to the thermodynamic and transport characterization of this phase.

8:12AM V34.00002 Quasiparticle interference above and below $T_c$ in underdoped cuprates \cite{1}. AAKASH PUSHP, COLIN PARKER, ABHAY PASUPATHY, KENJIRO GOMES, Princeton University, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, JINSHENG WEN, ZHUJIN XU, GENDA GU, Brookhaven National Laboratory, ALI YAZDANI, Princeton University — There is considerable debate over the evolution of quasiparticle excitations between the superconducting and pseudogap phases in the underdoped cuprates. In the superconducting phase, dispersive real space modulations are observed \cite{1}, which can be explained by quasi-particle interference (QPI), whose location in momentum space is consistent with ARPES. What should happen to these modulations in the pseudogap state, where ARPES indicates a finite arc of gapless Fermi surface? We will present STM data from underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ that investigates the nature of this change and its connection with the non-dispersive features seen above $T_c$ \cite{2}. [1] Kohsaka et al. Nature 454, 1072 (2008). [2] Vershchin et al. Science 305, 1993 (2004).

8:24AM V34.00003 Extinction of quasiparticle interference in underdoped cuprates with coexisting order. BRIAN ANDERSEN, University of Copenhagen, PETER HIRSCHELF, University of Florida — Recent scanning tunnelling spectroscopy measurements [Y. Kohsaka et al., Nature 454, 1072 (2008)] have shown that dispersing quasiparticle interference peaks in Fourier transformed conductance maps disappear as the bias voltage exceeds a certain threshold corresponding to the coincidence of the contour of constant quasiparticle energy with the antiferromagnetic zone boundary. Here we argue that this is caused by quasistatic short-range coexisting order present in the d-wave superconducting phase, and that the most likely origin of this order is disorder-induced incommensurate antiferromagnetism. We show explicitly how the peaks are extinguished in the related situation with coexisting long-range antiferromagnetic order, and discuss the connection with the realistic disordered case. Since it is the localized quasiparticle interference peaks rather than the underlying antinodal states themselves which are destroyed at a critical bias, our proposal resolves a conflict between scanning tunneling spectroscopy and photoemission regarding the nature of these states.

8:36AM V34.00004 Quasiparticle interference and vortex “checkerboard” in $\text{Bi}_2\text{Sr}_2\text{Ca}_0.8\text{Y}_{0.2}\text{Cu}_2\text{O}_y$. T. HANAGURI, Y. KOHSAKA, RIKEN, T. TAMEGAI, Univ. Tokyo, H. TAKAGI, RIKEN, Univ. Tokyo — Relationship between the “checkerboard” electronic modulation in a vortex core \cite{1} and the quasiparticle interference effect has been studied using STM/STS in optimally- doped $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{O}_8$. We found that the vortex- induced signals in Fourier-transform spectroscopic images appear in the close vicinity to some of the “octet” scattering vectors for the quasiparticle interference \cite{2}, suggesting that the vortex “checkerboard” is associated with the Fermi momentum. Conductance spectrum taken at the center of the vortex core shows a sharp peak at a low energy (~meV) in the empty state. We argue the possible relationship between these observations and the quantum-limit nature of the vortex core. [1] J. E. Hoffman et al., Science 295, 466 (2002). [2] K. McElroy et al., Nature 422, 592 (2003).

8:48AM V34.00005 Quasiparticle scattering from impurities in the cuprates, E.A. NOWADNICK, I.M. VISHIK, B. MORITZ, W.S. LEE, Z.X. SHEN, T.P. DEVEREAUX, Stanford University and SLAC, K. TANAKA, Osaka University — Scanning tunneling spectroscopy (STS) measurements have shown that the local density of states in the cuprate superconductors is spatially inhomogeneous. Fourier-transformed STS has been used to investigate the mixing of momentum space eigenstates of the superconducting quasiparticles in the presence of this inhomogeneity, and has observed the extinction of the quasiparticle peaks upon approaching the antinodal region of the Fermi surface. We present calculations of momentum dependent quasiparticle scattering from impurity sites. Our results demonstrate that the quasiparticle extinction observed in FT-STS can be interpreted as resulting from the momentum dependence of the quasiparticle scattering rather than the absence of the quasiparticle itself. This interpretation agrees with recent ARPES measurements that observe quasiparticle peaks over the entire Fermi surface.

9:00AM V34.00006 Echolocation of Scatterers by Quasiparticles in Cuprate Superconductors, SUMIRAN PUJARI, CHRISTOPHER HENLEY, Cornell University — How much can STM techniques tell us about the realization of disorder in a particular sample under study? We propose a new method of STM-data analysis which allows for the determination of the position and strength of impurities/scatterers. Furthermore, for cuprates, it can potentially be used to distinguish if the scatterer is “ordinary” or “anomalous” \cite{1}, i.e. part of the pairing potential. The method relies on quasiparticle interference \cite{2}[as observed in cuprates \cite{3}]. As for much of the STM phenomenology in cuprates \cite{1-3}, our starting point is the existence of well-defined Bogoliubov quasiparticles defined by a quadratic phenomenological Hamiltonian with intrinsic disorder. By Energy “Fourier-Transforming” the measured local density of states (LDS) spectrum from a single point, one can extract the “echo” time that a quasiparticle takes to go to and return from a nearby scatterer; doing this at several points in a local patch allows a “sonar”–like echolocation of the scatterer. This method is complementary to Fourier-Transform Scanning Tunneling Spectroscopy \cite{4} wherein Space Fourier transforms of LDS data yield the quasiparticle dispersion.

9:12AM V34.00007 Interference of nematic quantum critical quasiparticles: a route to the octet model. EUN-AH KIM, Cornell University, MICHAEL LAWLER, Binghamton University & Cornell University — Given the presence of glassiness and inhomogeneity in cuprate superconductors, the capability of quasiparticle interference (QPI) in inferring momentum space electronic structure from real space local density of states(LDOS) images is surprising. Particularly, the simplicity of the QPI image, a set of well defined dispersing peaks is striking. Regarding the nature of QPI peaks, the “octet model” was based on the observation that the peak positions are determined by the eight tips of the “banana” shaped qp energy contours. However, a key open question has the mechanism for the accumulation of coherence at the tips. Here we show that nematic quantum critical fluctuations, combined with the known extreme velocity anisotropy, provide a natural mechanism for the accumulation of coherence at those special points \cite{1}. Our results raise the intriguing question of whether the nematic fluctuations provide the unique mechanism for such a phenomenon.

9:24AM V34.00008 Tunneling-mediated Impurity Resonances in Bilayer Cuprate Superconductors, DEGANZ ZHANG, CHIN-SEN TING, Texas Center for Superconductivity and Department of Physics, University of Houston, TX 77204 — We have studied tunneling-mediated local density of states (LDOS) of the surface layer of a bilayer cuprate, where a Zn impurity is located on the second Cu-O layer. When the tunneling strength between two Cu-O layers is larger than a critical value, the LDOS on the site just above the Zn impurity first exhibits a resonant peak near the Fermi surface. The larger the tunneling strength, the stronger the resonant peak. It is also shown that the height of the resonant peak oscillates decreasingly with the distance from the site just above the Zn impurity. The location of the resonant peak in the surface LDOS depends on doping, energy gap, and the tunneling strength, and has an opposite bias voltage to that on its nearest neighboring sites. The results could be tested by the STM experiments and be used to further understand the electronic properties of high temperature superconductors.

9:36AM V34.00009 Spin Filtering and Dephasing through an Aluminum Nanoparticle, FELIPE TTIWA BIRK, Georgia Institute of Technology, CHRISTOPHER MALEC, Georgia Institute of Technology, DRAGOMIR DAVIDOVIC, Georgia Institute of Technology — Measurements of spin-polarized current through a single Al nanoparticle in weak tunnel contact with two ferromagnets will be discussed. As a function of the bias voltage across the particle, spin polarized current saturates within the first few discrete energy levels above the ground state. The saturation is related to the energy dependence of the spin relaxation time \( T_1 \), from which we find that \( T_1 \) is about microsecond for the lowest excited state. Spin polarized current is extremely sensitive with respect to the direction of the applied magnetic field relative to magnetization. The discrete levels filter the spin of transmitted electrons along the direction specified by the applied magnetic field, explaining the directional dependence both qualitatively and quantitatively. In zero magnetic field, the filtering direction is determined by the field of the environment, making spin-filtering a new technique to study electron spin-dephasing in single metallic particles and other quantum dots. The spin-dephasing time in the nanoparticle at 4.2K is \( T_2 \gg 8\mu s. \)

9:48AM V34.00010 Possible competing order-induced Fermi arcs and self-consistent gap evolution with temperature in cuprate superconductors, G.P. LOCKHART, A.D. BEYER, M.L. TEAGUE, B.-L. YU, J.C.F. WANG, N.-C. YEH, Physics Dept., Caltech, Pasadena, CA — We explore, via numerical simulations, the possibility that competing orders (CO’s) induce both the pseudogap (PG) and Fermi arc phenomena in cuprate superconductors. We find that both phenomena occur in hole-type cuprates if (1) a CO arises below a FG PG temperature, \( T^\ast \), which is greater than the superconducting transition temperature, \( T_C \), and (2) the periodic wave-vector of the CO, \( Q \), is parallel to the Cu-O bonding direction. In contrast, neither phenomena is observed in electron-type cuprates because \( T^\ast < T_C \), but we find evidence that the CO scenario may explain the so-called non-monotonic d-wave gap observed in electron-type cuprates for \( T^\ast < T_C \) if \( Q \) is parallel to the nodal direction, as in the case of commensurate spin density waves. Finally, we consider a candidate model for self-consistently calculating the superconducting and CO energy gaps as a function of temperature and doping in the hole-type cuprates, as well as estimating the value of \( T^\ast \). Ref.: B.-L. Yu, et al. [arxiv:0804.4028].

10:00AM V34.00011 How does the gap change at \( T_C \) in underdoped cuprates?, COLIN PARKER, AAKASH PUSHP, ABHAY PAPASUTHY, Princeton University, KENJIRO GOMES, SHIMPEI ONO, CRIEPI, Japan, YOICHI ANDO, ISIR, Osaka University, JINSCHENG WEN, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, ALI YAZDANI, Princeton University — Many measurements on underdoped cuprates have shown a gap that persists up to room temperature. This raises an important question: what happens at \( T_C \) in order to cause the loss of perfect conductivity? In ARPES, the nature of the gap changes from d-wave below \( T_C \) to Fermi arcs above \( T_C \). However, ARPES necessarily averages over significant nanoscale disorder. We will present detailed STM spectroscopy on underdoped \( Bi_2Sr_2CuO_4 \) single crystals both above and below \( T_C \). Unlike overdoped samples, the STM spectrum in underdoped cuprates shows two energy scales [1]. We will compare our data to models based on ARPES, with emphasis on the difference between the superconducting and pseudogap phases. [1] Gomes et al., Nature 447, 569 (2007) [2] Pasupathy et al., Science 320, 196 (2008)

1Work supported by DOE, PCCM-MRSEC.

10:12AM V34.00012 The Effect Of Spontaneous Magnetization On The Reliability Of The Value For The Spin Polarization As Fitted From Ferromagnet/Superconductor Point Contact Data, PAUL J. DOLAN, JR., Northeastern Illinois University, CHARLES W. SMITH, University of Maine — The generalized BTK model for charge transport in a ferromagnet/superconductor point contact can be used to estimate the spin polarization in a ferromagnet. However, even when these measurements are carried out in zero applied magnetic field, there can be a substantial field in the active region of the contact due to the spontaneous magnetization of the ferromagnet itself. We estimate the effect of spontaneous magnetization on the reliability of the value of the spin polarization parameter for various ranges in contact transparency, inelastic scattering and temperature.

10:24AM V34.00013 Coherence factor effects in the antisymmetrized LDOS correlators, MARI-ANNA MALTSEVA, Dept of Physics and Astronomy, Rutgers University, P. COLEMAN, Dept Physics and Astronomy, Rutgers University — Recent scanning tunneling experiments on underdoped cuprates by Hanaguri et al [1] show the appearance of coherence factor effects. Unlike conventional observables, we show that the tunneling density of states in a superconductor does not have a well defined coherence factor. However, by extracting the component that is either even, or odd in the bias voltage, we show that these separate components have well-defined coherence factors. These results are used to understand the appearance of coherence factor effects in the antisymmetrized local density of states correlators in recent scanning tunneling experiments.


1Supported by DMR NSF-0605935.

10:36AM V34.00014 Visualizing electronic segregation in lightly-doped \( Ca_{2-x}Na_xCuO_2Cl_2 \). YUKI KOHSAKA, TETSUO HANAGURI, RIKEN, MASAKI AZUMA, MIKIO TAKANO, Tokyo Univ., J. C. SEAMUS DAVIS, Cornell Univ., HIDENORI TAKAGI, RIKEN/Univ. of Tokyo — We report spectroscopic imaging on evolution of the electronic state in a lightly-doped cuprate superconductor \( Ca_{2-x}Na_xCuO_2Cl_2 \) across the metal-insulator critical doping. We find nm-scale electronic segregation between regions breaking and showing the lattice symmetry. The former shows \( C_2 \) symmetry characterized by the unidirectional nano-domains and the V-shaped pseudogap found in superconducting samples [1] while the latter shows \( C_3 \) symmetry and wider U-shaped gap prominent in non-superconducting samples. This indicates that the local symmetry breaking is inherent in the electronic states created inside the Mott gap by hole doping. We also discuss spectra in \( C_2/C_3 \) domains and superconducting/insulating samples.

describe the consequences of this for the Leggett mode and outline possible experimental signatures of this sign difference between the two superconducting gaps. Unlike previously studied systems, in this model the superconducting order parameters of the particle and hole Fermi surfaces naturally have opposite sign. We calculate the spectrum of this mode in a short-range exchange model of iron pnictide superconductors. We analyze the implications of our results with experimental data for Fe-pnictides, where such a sign-changing $s$-wave state may be realized. We consider a phenomenological model for sign changing $s$-wave order parameters appropriate for the ferropnictide superconductors. We compare our results with experimental data for Fe-pnictides.

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Thursday, March 19, 2009 8:00AM - 10:48AM –

Session V35 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors XIII: Pairing Symmetry, Theory and Experiment  405

8:00AM V35.00001 On the magnetic fluctuations and unconventional superconducting pairing in iron pnictides 1, JINHUA ZHANG, RASTIKO SKNEPNKE, JOERG SCHMALIAN, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — We explore the role played by spin and density fluctuations in the FeAs based superconductors using the fluctuation-exchange (FLEX) approach. We calculate the superconducting transition temperature and the fluctuation induced pairing gap. In order to compare with experiments, we evaluate the change of the penetration depth with temperature and the evolution of the order parameter. Because of the multi-band feature in this type of material, the interplay between intra- and inter-band fluctuations gives rise to rich physics.

1Supported by the U.S. Department of Energy Contract No. DE-AC 02-07CH11358.

8:12AM V35.00002 Signatures of the $s^+$ superconducting gap in electronic Raman Scattering and optical conductivity of Fe-based superconductors  , ILYA EREMIN, MPI for Physics of Complex Systems, ANDREY V. CHUBUKOV, MAXIM M. KORSHUNOV — We analyze the consequences of the extended $s$-wave symmetry of the superconducting gap, proposed recently in Fe-based superconductors, for the electronic pairing Raman scattering and optical conductivity. We calculate conductivity and Raman intensity for elastic scattering and find that an extended $s$-wave superconducting gap gives rise to several specific features in optical and Raman response functions. In particular, we find that, for the $A_{1g}$ symmetry of the incoming light, there will be a resonant collective mode in the Raman response function at an energy $\omega < 2\Delta$. The latter is as a hallmark of the $s^+$ superconductivity. Furthermore, the Cooper-pair weakening due to strong inter-band impurity scattering shifts the $2\Delta$ features towards higher energies in both Raman scattering and optical conductivity. We argue that these features are present in the experimental data for iron-based superconductors.

8:24AM V35.00003 Experiments for probing the macroscopic quantum coherence and pairing state in FeAs-based superconductors  , C.C. TSUEI, CHING-TZU CHEN, M.B. KETCHEN, IBM T.J. Watson Research Center, Z.A. REN, Z.X. ZHAO, Chinese Academy of Sciences, Beijing, China, X.H. CHEN, University of Science and Technology of China, Anhui, China — The recent discovery of superconductivity in FeAs-based pnictides has added another member to the growing family of high-temperature superconductors. In sharp contrast to cuprates, the new superconductor has a $T_c$ up to 55 K despite the absence of strong electronic correlation. Furthermore, its physical properties are best described by the multi-orbital electronic band structure. It is therefore of great interest to explore the consequences of these novel characteristics on the nature of Cooper pairing in the new Fe As superconductors. In this talk, we will present the design and implementation of experiments which probe the pairing state and the macroscopic quantum coherence across the interface between a pnictide and a conventional $s$-wave superconductor. Preliminary results will be discussed.

8:36AM V35.00004 Limits on the Superconducting Order Parameter in NdFeAsO$_{1−\delta}$F$_y$ and SmFeAsO$_{1−\delta}$ From Scanning SQUID Microscopy  , THOMAS LIPPMAN, CLIFFORD HICKS, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California, 94305, USA, MARTIN HUBER, Department of Physics and Electrical Engineering, University of Colorado Denver, Denver, Colorado, 80217, USA, ZHI-AN REN, ZHONG-XIAN ZHAO, National Laboratory for Superconductivity, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, P.R. China, KATHRYN MOLER, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, California, 94305, USA — As a test of the symmetry of the order parameter of the ferric oxyarsenide family of superconductors $R$FeAsO$_{1−\delta}$F$_y$, where $R$ is a rare earth, we perform scanning SQUID microscopy on dense polycrystalline samples of NdFeAsO$_{0.94}F_{0.06}$ and SmFeAsO$_{0.85}$. Dominant $d$- or $p$-wave orders, for example, would result in direction-dependent phase shifts in tunneling. In well-coupled polycrystalline samples, these phase shifts would result in spontaneous orbital currents and magnetization in the superconducting state. We do not find any spontaneous currents in NdFeAsO$_{0.94}F_{0.06}$ or SmFeAsO$_{0.85}$, ruling out order parameters with direction-dependent phase shifts in tunneling.

8:48AM V35.00005 Effect of disorder on sign reversing s-wave pair state for Fe-pnictides  , VIVEK MISHRA, G. BOYD, S. GRASER, P. J. HIRSCHFELD, Department of physics,University of Florida, Gainesville, FL-32611,USA. — In this work, we consider a phenomenological model for sign changing s-wave order parameters appropriate for the ferropnictide superconductors. We consider both magnetic and non-magnetic impurities within the Born approximation, and study the effects of this disorder on transport properties in superconducting state. Our results can be used to guide experiments and design Fe-pnictides.

9:00AM V35.00006 Phase fluctuations in a magnetic exchange model of iron-based superconductors  , F.J. BURNELL, Princeton University, B. ANDREI BERNEVIG, MEERA M. PARISH, Princeton Center for Theoretical Science — We analyze the phase fluctuations in a two band model of iron-based superconductors. Multi-band superconductors have a sound-like collective excitation (Leggett mode) due to phase oscillations between different condensates. We calculate the spectrum of this mode in a short-range exchange model of iron pnictide superconductors. Unlike previously studied systems, in this model the superconducting order parameters of the particle and hole Fermi surfaces naturally have opposite sign. We describe the consequences of this for the Leggett mode and outline possible experimental signatures of this sign difference between the two superconducting gaps.
9:12AM V35.00007 Near degeneracy of several pairing channels in a multi-orbital model for the Fe-pnictides. THOMAS MAIER, Oak Ridge National Laboratory, SIEGFRIED GRASER, PETER HIRSCHFELD, University of Florida, DOUGLAS SCALAPINO, University of California, Santa Barbara — The experimental evidence regarding the gap structure in different iron pnictide superconductors is currently conflicting. In addition, weak-coupling approaches to the pairing problem in multi-orbital models of the iron pnictides have predicted a wide variety of superconducting ground states. We argue here that this controversy is naturally explained by the near-degeneracy of different pairing channels in superconductors with many distinct Fermi surface sheets. In particular, we will present results for the spin susceptibility and the pairing symmetry within a five-band random phase approximation model. We will discuss the robustness of these results for different dopings, interaction strengths, and variations in the band structure, in the light of recent experiments.

9:24AM V35.00008 Pairing Symmetry in a Two-Orbital Exchange Coupling Model of Oxypnictides. B. ANDREI BERNEVIG, Princeton University, KANGJUN SEO, JIANGPING HU — We study the pairing symmetry of a two orbital $J_1 - J_2$ model for FeAs layers in oxypnictides. We show that the mixture of an intra-orbital unconventional $s_{+2} \sim \cos(k_x) \cos(k_y)$ pairing symmetry and a small $d_{x^2-y^2}$ component is favored in a large part of $J_1 - J_2$ phase diagram. A pure $s_{+2}$ pairing state is favored for $J_2 \gg J_1$. The signs of the $d_{x^2-y^2}$ order parameters in the two different orbitals are opposite. While a small $d_{x^2-y^2} \sim \sin(k_x) \sin(k_y)$ inter-orbital pairing coexists in the above phases, the intra-orbital $d_{x^2-y^2}$ pairing is not favored even for large $J_2$.

9:36AM V35.00009 Self-consistent calculations of the local density of states of FeAs superconductor/ferromagnet bilayers. NAYOUNG LEE, HAN-YONG CHOI, SungKyunKwan University — We study the local density of states (L DOS) of the superconductor/ferromagnet (S/F) bilayers using the self-consistent Bogoliubov-de Gennes equation, where the S is modeled in terms of the $s+\pi$ pairing state. The $s+\pi$ pairing is an $s$-wave pairing state with an internal $\pi$ phase between the two condensates of a two band superconductor which seems relevant for the FeAs superconductors. We calculate the pairing and magnetic order parameters self-consistently to obtain LDOS as a function of the energy and position of S/F bilayers. The results will be discussed in terms of the interplay between the internal and external $\pi$ phases.

9:48AM V35.00010 Possible time-reversal symmetry breaking pairing state in FeAs superconductors. WEI-CHENG LEE, University of California, San Diego, SHOU-CHENG ZHANG, Stanford University, CONJUN WU, University of California, San Diego — We investigate the consequences of the intra-band $s$-wave and $d$-wave pairing order parameters in the iron-based superconductors. Because of the frustrating pairing interactions among the electron and the hole Fermi pockets, a time reversal symmetry breaking $s+id$ pairing state could be favored. We analyze this pairing state within the Ginzburg-Landau theory, and explore the experimental consequences. In such a state, spatial inhomogeneity induces supercurrent near a non-magnetic impurity and the corners of a square sample. The resonance mode between the $s$ and $d$-wave order parameters can be detected through the $B_{1g}$-Raman spectroscopy.

10:00AM V35.00011 Spin fluctuation mediated extended s-wave pairing from multiple Fermi surfaces in iron pnictide superconductors. KAZUHIKO KUROKI, Department of Applied Physics and Chemistry, The University of Electro-Communications and JST, TRIP, SEICHIRO ONARI, Department of Applied Physics, Nagoya University and JST, TRIP, RYOTARO ARITA, Department of Applied Physics, University of Tokyo and JST, TRIP, HIDETOMO USUI, Department of Applied Physics and Chemistry, The University of Electro-Communications and JST, TRIP, YUKIO TANAKA, Department of Applied Physics, Nagoya University and JST, TRIP, HIROSHI KONTANI, Department of Physics, Nagoya University and JST, TRIP, HIDEKO AOKI, Department of Physics, University of Tokyo and JST, TRIP — For the superconducting iron pnictides, we have constructed a minimal model, where all the five Fe d bands turn out to be involved. We study the fluctuation dynamics of these superconducting states, as well as d- and p-wave states. The coupling between spin fluctuations and the quasiparticles of the superconducting state leads to damping of the former. The gap structure leaves a signature in the form of this damping. This can be used to diagnose the order parameter in spin sensitive experiments. We also discuss the case of coexistence of superconductivity and spin-density wave.

10:12AM V35.00012 Spin fluctuation dynamics and multiband superconductivity in iron pnictides. VALENTIN STANEV, JIAN KANG, ZLATKO TESANOVIC, Johns Hopkins University — Multiband superconductivity, involving resonant pair scattering between different bands, has emerged as a likely possibility for the iron pnictides. In this scenario the gap changes sign between the hole and the electron Fermi surfaces (separated by wave-vector M). In the quest to distinguish this extended s- from an ordinary s- wave state, it is essential to use experiments that have momentum space resolution and can probe momenta of order M. We study the fluctuation dynamics of these superconducting states, as well as d- and p-wave states. The coupling between spin fluctuations and the quasiparticles of the superconducting state leads to damping of the former. The gap structure leaves a signature in the form of this damping. This can be used to diagnose the order parameter in spin sensitive experiments. We also discuss the case of coexistence of superconductivity and spin-density wave.

1. Research supported in part by the NSF under Grant No. DMR-0531159 and by the DOE under Grant No. DE-FG02-08ER46544


10:24AM V35.00013 Emergent symmetry of superconductivity and antiferromagnetism in the iron pnictides. YONG BAEK KIM, DANIEL PODOLSKY, HAE-YOUNG KEE, University of Toronto — We show the presence of an emergent symmetry that unifies superconductivity and magnetism in the iron pnictides. We discuss the expected experimental consequences of this symmetry.

10:36AM V35.00014 Two-band Model for Unconventional Superconductivity in Iron-Based Superconductors. YAN CHEN, (1) Dept. of Physics and Lab of Advanced Materials, Fudan University (2) Texas Center for Superconductivity, University of Houston — The recent discovery of FeAs superconductors with high Tc has triggered intensive efforts to explore magnetism and superconductivity in this family of materials. We adopt an effective model Hamiltonian including a two-band tight-binding term as well as a spin-spin exchange interaction term. The first term can fit approximately the multi-band dispersions near electron/hole Fermi-pockets while the second term may lead to the appropriate superconducting pairing symmetry as well as the SDW state at low doping. Different pairing symmetry candidates of FeAs materials are evaluated for various model parameters. In particular, we study the local electronic structure at vortex cores in the system subject to an external magnetic field. The relevance to recent STM measurements will be discussed. Moreover, we calculate the tunneling conductance of various superconducting junctions, including the Josephson current in the superconducting state. The Josephson current can be decomposed into two parts, an interband and an intraband component. Distinct interference effects can be used to distinguish the pairing symmetry of FeAs systems.
8:12AM V37.00002 Nonlinear Response Functions in Model Dissipative Anharmonic Systems

MOHAMMAD SAHRAPOUR, NANCY MAKRI, University of Illinois at Urbana-Champaign — We report the results of simulations of third order response functions \( R^{(3)}(\tau_1, 0, \tau_1) = \text{Tr} \left( \hat{\alpha}(\tau_1) \hat{\alpha}(\tau_1) \hat{\alpha}(\tau_1) \right) \) where \( \hat{\alpha} \) is the polarizability for harmonic, Morse, and anharmonic model systems in a linearly dissipative environment. These simulations are carried out via the iterative path integral methodology developed earlier in our group which delivers efficient, numerically exact long time quantum dynamics. We find that even minor anharmonicity in the potential qualitatively changes the response function; rotating the pattern seen by 45° in the \( \tau_1 - \tau_3 \) plane. We also observe that modulations in the \( \tau_2 \) direction increase in frequency as we go to a more anharmonic potential. As the temperature is increased, these modulations also appear in the \( \tau_1 \) direction. It is also found that asymmetry in the potential, at least at temperatures considered here, does not have a significant effect. Finally, in all three systems we notice that decay in the \( \tau_2 \) direction is faster than in the \( \tau_1 \) direction. The observed sensitivity of the response function to anharmonicities in the potential can be exploited to construct more accurate molecular potentials once the appropriate non-linear spectroscopic experiments have been performed.

8:24AM V37.00003 Hamiltonian Monodromy: Unexpected behavior of quasi-linear molecules, atoms in traps and of hydrogen in crossed fields

J.B. DELOS, William and Mary, C. SCHLEIF, UC Merced, D. SADOVSKII, G. DHONT, B. ZHILINSKII, U. du Littoral — A system exhibits monodromy if we take the system around a closed loop in its parameter space, and we find that the system does not come back to its original state. Many systems have this property, including quasi-linear molecules, atoms in a trap or a hydrogen atom in crossed fields. Using classical perturbation theory, Sadowski and Cushman predicted the presence of monodromy in perpendicular fields. It shows up as a defect in the lattice of quantum states. When the fields are tilted from perpendicular, this lattice defects undergo a series of bifurcations. Atoms in a trap can display a newly discovered dynamical manifestation of monodromy. This phenomenon will also occur with oriented dipolar molecules in fields or with quasilinear molecules. (Supported by NSF and Region Nord–Pas-de-Calais)

8:36AM V37.00004 On the internal photorelaxation mechanism of DNA

JESSICA A. THOMAS, LEONARDO ALVAREZ-VALTIERRA, DAVID W. PRATT, University of Pittsburgh — Gas phase rotationally resolved electronic spectra were collected for the origin and several vibronic transitions of 1,3-benzodioxole. For each band, an autocorrelation function \( \alpha(\tau_1, 0, \tau_0) = \text{Tr} \left( \hat{\alpha}(\tau_1) \hat{\alpha}(\tau_1) \right) \) where \( \hat{\alpha} \) is the polarizability) for harmonic, Morse, and anharmonic model systems in a linearly dissipative environment. These simulations are carried out via the iterative path integral methodology developed earlier in our group which delivers efficient, numerically exact long time quantum dynamics. We find that even minor anharmonicity in the potential qualitatively changes the response function; rotating the pattern seen by 45° in the \( \tau_1 - \tau_3 \) plane. We also observe that modulations in the \( \tau_2 \) direction increase in frequency as we go to a more anharmonic potential. As the temperature is increased, these modulations also appear in the \( \tau_1 \) direction. It is also found that asymmetry in the potential, at least at temperatures considered here, does not have a significant effect. Finally, in all three systems we notice that decay in the \( \tau_2 \) direction is faster than in the \( \tau_1 \) direction. The observed sensitivity of the response function to anharmonicities in the potential can be exploited to construct more accurate molecular potentials once the appropriate non-linear spectroscopic experiments have been performed.

8:48AM V37.00005 Tunneling Splitting in the Rotationally Resolved Electronic Spectrum of 1,3-Benzodioxole

TUNELLA, DAVID W. PRATT, University of Pittsburgh — Gas phase rotationally resolved electronic spectra were collected for the origin and several vibronic transitions of 1,3-benzodioxole. For each band, an autocorrelation function \( \alpha(\tau_1, 0, \tau_0) = \text{Tr} \left( \hat{\alpha}(\tau_1) \hat{\alpha}(\tau_1) \right) \) where \( \hat{\alpha} \) is the polarizability) for harmonic, Morse, and anharmonic model systems in a linearly dissipative environment. These simulations are carried out via the iterative path integral methodology developed earlier in our group which delivers efficient, numerically exact long time quantum dynamics. We find that even minor anharmonicity in the potential qualitatively changes the response function; rotating the pattern seen by 45° in the \( \tau_1 - \tau_3 \) plane. We also observe that modulations in the \( \tau_2 \) direction increase in frequency as we go to a more anharmonic potential. As the temperature is increased, these modulations also appear in the \( \tau_1 \) direction. It is also found that asymmetry in the potential, at least at temperatures considered here, does not have a significant effect. Finally, in all three systems we notice that decay in the \( \tau_2 \) direction is faster than in the \( \tau_1 \) direction. The observed sensitivity of the response function to anharmonicities in the potential can be exploited to construct more accurate molecular potentials once the appropriate non-linear spectroscopic experiments have been performed.

9:00AM V37.00006 Vacuum Ultraviolet Absorption of Supercritical Water

DAVID BARTELS, IRENEUSZ JANIK, Notre Dame University, TIMOTHY MARIN, Benedictine University — The first continuum \( \sim \) peak in the gas phase absorption spectrum of H$_2$O (maximum at 7.4 eV), is ascribed to promotion of a nonbonding valence electron to a dissociative excited state which is an admixture of antibonding sigma and 3s Rydberg orbitals. Due to the large spatial extent of this orbital the \( \sim \) peak is strongly perturbed by the local environment. In liquid water, this peak is notably broadened and shifted to the blue, with an absorption maximum of 8.3 eV at room temperature. An obvious question is how this transition changes as a function of the water density in the supercritical regime as the system transitions from liquid to gas. As density decreases, most water molecules form hydrogen bonds. When the fields are tilted from perpendicular, this lattice defects undergo a series of bifurcations. Atoms in a trap can display a newly discovered dynamical manifestation of monodromy. This phenomenon will also occur with oriented dipolar molecules in fields or with quasilinear molecules. (Supported by NSF (CHE-0615755))
9:24AM V37.00008 Ab Initio Torsion-Wag Surface for the Ethyl Radical\(^1\), RAM S. BHATTA, DAVID S. PERRY, Department of Chemistry, The University of Akron — The torsion-wag potential of the ethyl radical has a 6-fold barrier to internal rotation and the minimum energy path involves deviations of the \(\text{CH}_2\) wag angle of 6 to 11 degrees on either side of planar. Partially optimized 2-dimensional surfaces were calculated at the B3LYP, MP2, and CCSD(T) levels with 6-311++G(d,p) and 6-311++G(3df, 2p) basis sets and they were fit to a function containing a polynomial in the wag angle \(\tau\) and trigonometric functions of the torsional angle \(\alpha\). Comparison is made with the corresponding surfaces for \(\text{CH}_3\text{NH}_2\) and \(\text{CH}_3\text{OH}\). Unlike \(\text{CH}_2\text{CH}_2\), both have a substantial barrier to inversion. The dominant torsion-wag coupling term in all three cases has the form \(\tau \cos \alpha\).

\(^1\)The work was supported by the Office of Basic Energy Sciences, Office of Energy Research, U.S. Department of Energy under Grant No. DE-FG02-90ER14151.

9:36AM V37.00009 Terahertz Investigations of Extraordinarily Efficient Conduction in a Redox Active Ionic Liquid. VERNER THORSMOLLE, JAN BRAUER, Ecole Polytechnique Federale de Lausanne, GIDRO ROTHENBERGER, Polytechnique Federale de Lausanne, DAIBIN KUANG, Sun Yat-Sen University, SHAIK ZAKEERUDDIN, MICHAEL GRÄTZEL, JACQUES MOSER, Polytechnique Federale de Lausanne — In this talk, we will present our terahertz investigations of extraordinary charge transport in a redox-active ionic liquid, namely [\(\text{C}_{18}\text{H}_{37}\text{N}_{14}\text{S}_{6}\text{O}_{5}\)]\(^{2+}\)\((\text{DO}_{2})_2\)\(^{2-}\) in \(\text{CH}_{3}\text{OH}\). The redox-active ionic liquid shows a high conductivity of \(10^{-3}\) S/cm at room temperature, which is comparable to other reports on redox-active ionic liquids. Our terahertz investigations reveal that the charge transport in this ionic liquid is dominated by the redox-active \(\text{C}_{18}\text{H}_{37}\text{N}_{14}\text{S}_{6}\text{O}_{5}\)^{2+} cations, which show a reaction field relaxation time of \(\tau_r = 540\) fs. This relaxation time is much shorter than the thermal relaxation time, which suggests that the charge transport is driven by a reaction field relaxation mechanism. The ionic liquid retains its conductivity in a high pressure environment up to \(15\) GPa, and a high pressure phase transition is observed at \(9.3\) GPa, which is accompanied by a decrease in the conductivity.

9:48AM V37.00010 Investigation of the Order-Disorder Transition in the Hybrid Inorganic-Organic System [(\text{CH}_3)_2\text{NH}]_2\text{Zn(HCOO)}_2, by means of \(^1\)H NMR. T. BESARA, P. JAIN, Department of Chemistry, Florida State University, Tallahassee, FL, USA, A.P. REYES, P.L. KUHN, National High Magnetic Field Laboratory, Tallahassee, FL, USA, A.K. CHEETHAM, Materials Research Laboratory, University of California, Santa Barbara, CA, USA — [(\text{CH}_3)_2\text{NH}]_2\text{Zn(HCOO)}_2, a hybrid ABX\(_3\) perovskite, with A=(\text{CH}_3)_2\text{NH}, B=Zn and X=HCOO, undergoes a paraelectric-antiferroelectric transition around 156 K. Synchrotron studies indicate that hydrogen bonding between the H-atoms in the NH\(_2\) group and O-atoms from the formate group is involved. The dimethylethylamine cation is ordered with nitrogen existing in three different positions, but not known whether statically or dynamically. We have investigated it by means of Spin-lattice relaxation time, \(T_1\), using proton NMR. We find that the cation is dynamically disordered and that the transition involves its slowing down. Evidence is seen for tunneling of the CH\(_2\) groups, and for the compound becoming a glass, with the cation displaying several metastable equilibrium geometries (\(T_1\) trajectories).

10:00AM V37.00011 High Resolution Cavity Ringdown Spectroscopy of Jet-Cooled Reactive Intermediates, GABRIEL JUST, PATRICK RUPPER, LINSEN PEI, TERRY MILLER, The Ohio State University — Alkyl peroxy radicals long have been well known to be key intermediates in atmospheric and chemistry as well as in low-temperature combustion. For the last several years, our group has generated a data set for these radicals using room-temperature cavity ringdown spectroscopy. We have recently extended our investigations of the peroxy radicals to obtain a high-resolution data set of spectra under jet-cooled conditions using a quasi-Fourier-transform-limited laser source and a supersonic slit jet discharge expansion. Over the last few years, we have developed our capability to obtain narrow-bandwidth, near-infrared (NIR) radiation for performing high-resolution cavity ringdown spectroscopy using the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser. The NIR light can be generated by either stimulated Raman shifting or by working in the post-amplification of a Ti:Sa ring laser.
Observation of the $\tilde{A} - \tilde{X}$ Electronic Transitions of Cyclopentyl and Cyclohexyl Peroxy Radicals Via Cavity Ringdown Spectroscopy

The $\tilde{A} - \tilde{X}$ transitions of cyclopentyl and cyclohexyl peroxy radicals are important intermediates in combustion chemistry. These molecules, formed from the addition of oxygen to alkyl radicals, are pivotal species in many atmospheric processes. We have previously targeted the $\tilde{A} - \tilde{X}$ transitions of straight- and branched aliphatic peroxy radicals. This research has now been extended towards cyclic systems starting with cyclopentyl peroxy ($C_5H_9O_2$) and cyclohexyl peroxy ($C_6H_{11}O_2$), which are predicted by ab initio and DFT calculations to have four and two low-lying conformers respectively. Both have conformers which differ on the O-O bond with respect to the cyclic skeleton namely, cis- and gauche-, with $C_6H_{11}O_2$ also having conformers with axial and equatorial placement on the ring. We observe strong bands for both peroxies in the near-IR which are favorably assigned as the origin and the O-O stretch in agreement with the calculations. We have also obtained the spectrum of $C_6O_1D_2$ which facilitates the assignments of the weaker vibrational structure in $C_6H_{11}O_2$.

Dynamic light scattering in an aqueous solution of 3-methylpyridine

DIMITRY IVANOV, ANNA TRUBETSKAYA, University of Maryland, ANDREI KOSTKO, Virginia Commonwealth University, MIKHAIL ANISIMOV, JAN SENGERS, University of Maryland — We report a set of dynamic light scattering experiments in an aqueous solution of 3-methylpyridine. The dynamic correlation functions appear to exhibit two modes: one associated with a normal diffusion process and another one with network relaxation. The observed correlations seem to be associated with long-living nonequilibrium structures. To obtain further insight into this phenomenon we have made systematic studies of the nature of the observed dynamics as a function of time and concentration.

Quantum Transition State Theory

HOLGER WAALKENS — The main idea of Wigner’s transition state theory (TST) is to compute reaction rates from the flux through a dividing surface placed between reactants and products. In order not to overestimate the rate the dividing surface needs to have the no-crossing property, i.e. reactive trajectories cross the dividing surface exactly once, and nonreactive trajectories do not cross it at all. The long standing problem of how to construct such a dividing surface for multi-degree-of-freedom systems was solved only recently using ideas from dynamical systems theory. Here a normal form is available for a local decoupling of the classical dynamics which leads to the explicit construction of the phase space structures that govern the reaction dynamics through transition states. The dividing surface is spanned by a normally hyperbolic manifold which is the mathematical manifestation of the transition state as an unstable invariant subsystem of one degree of freedom less than the full system. The mere existence of a quantum version of TST is discussed controversially in the literature. The key issue is the presence of quantum mechanical tunneling which prohibits the existence of a local theory analogous to the classical case. Various approaches have been developed to overcome this problem by propagating quantum wavefunctions through the transition state region. These approaches have in common that they are computationally very expensive which seriously limits their applicability. In contrast the approach by Roman Schubert, Stephen Wiggins and myself is local in nature. A quantum normal form allows us to locally decouple the quantum dynamics to any desired order in Planck's constant. This yields not only the location of the scattering and resonance wavefunctions relative to the classical phase space structures, but also leads to very efficient algorithms to compute cumulative reaction probabilities and Gamov-Siegert resonances which are the quantum imprints of the transition state.

Transition States in a Noisy Environment

THOMAS BARTSCH, Loughborough University — No abstract available.

Statistical Theory of Asteroid Escape Rates

CHARLES JAFFE, Department of Chemistry, West Virginia University — Transition states in phase space are identified and shown to regulate the rate of escape of asteroids temporarily captured in circumplanetary orbits. The transition states, similar to those occurring in chemical reaction dynamics, are then used to develop a statistical semianalytical theory for the rate of escape of asteroids temporarily captured by Mars. Theory and numerical simulations are found to agree to better than 1%. These calculations suggest that further development of transition state theory in celestial mechanics, as an alternative to large-scale numerical simulations, will be a fruitful approach to mass transport calculations.

Exploring remnants of invariants buried in a deep potential well in chemical reactions

TAMIKI KOMATSUZAKI, Hokkaido University — How the reacting system climbs through saddles from one basin to another on potential energy surface has been one of the most intriguing subjects not only in chemistry but also physics and biology. This decade significant progress has been achieved in establishing the concept of the so-called transition state (TS), that is, a hypersurface of co-dimension one through which the system passes through only once from one basin to another [1-3]. However, there exist still open problems to be resolved; 1) how the no-return TS ceases or bifurcates as the energy increases [4, 5] or how one can generalize the concept of return TS besides the region of first-rank saddles. Related to the problem 2), most of all the chemical reaction theories assume that all of the available energy redistributes statistically through the dofs of system in the reactant well before the reaction takes place. It is implicitly expected that the ratio of the measure occupied by tori in phase space is that of the ambient space decreases exponentially as the dimensionality of the system increases. Here we present a novel technique to scrutinize the remnant of invariants buried in chaos in many-degrees of freedom systems [7]. This is regarded as the remnants of a destroyed invariant manifold that may dominate the transport in phase space even at high energy regions where most of all tori vanish. We demonstrate the potentiality of our technique for HCN isomerization, where the conventional procedure based on a finite order truncation in the coordinate transformation of canonical perturbation theory prevent us from detecting remnants of invariants.

1T.K. acknowledges financial support from JSPS and Grant-in-Aid for Research on Priority Area “Molecular Theory for Real Systems.”
from a much earlier study by De Leon and Berne. Nonlinear resonances and phase space traps which potentially result in quantum eigenstates of varying degree of localization.

3. Representation of the classical phase space (Arnol’d web) highlighting the important dynamical structures. Insights into the dynamics originate from the various energy flow in the system from both classical and quantum viewpoints. Using a wavelet-based local frequency analysis it is possible to construct a useful representation of a freedom. Several studies have established that such systems are prime candidates for observing non-RRKM behavior.

This talk focuses on a mechanistic understanding of the deviations from RRKM theory for a model isomerization problem with three degrees of freedom. Continuing efforts to characterize the phase space structure of systems with three or more degrees of freedom are beginning to yield crucial mechanistic insights.

Kassel-Marcus (RRKM) theory. Since both theories have classical dynamics at their foundation, advances in our understanding of nonlinear dynamics and chemical dynamics with researchers critically examining the validity of the two pillars of reaction rate theory - transition state theory and the Rice-Ramsperger-Kassel-Marcus (RRKM) theory. Since both theories have classical dynamics at their foundation, advances in our understanding of nonlinear dynamics and continuing efforts to characterize the phase space structure of systems with three or more degrees of freedom are beginning to yield crucial mechanistic insights into the dynamics. This talk focuses on a mechanistic understanding of the deviations from RRKM theory for a model isomerization problem with three degrees of freedom. Several studies have established that such systems are prime candidates for observing non-RRKM behavior.

The model is inspired, and generalized, from a much earlier study by De Leon and Berne. We try to answer two of the questions posed in this early work by studying the intramolecular vibrational energy flow in the system from both classical and quantum viewpoints. Using a wavelet-based local frequency analysis it is possible to construct a useful representation of the classical phase space (Arnol’d web) highlighting the important dynamical structures. Insights into the dynamics originate from the various nonlinear resonances and phase space traps which potentially result in quantum eigenstates of varying degree of localization.

This work was supported by ONR, NSF, DOE and HPCMO.

10:48AM V38.00007 Classical-Quantum correspondence in isomerization dynamics: quantum eigenstates and classical Arnol’d web. S. KESHAVAMURTHY, IIT Kanpur, India — Recently, there has been a renaissance of sorts in chemical dynamics with researchers critically examining the validity of the two pillars of reaction rate theory - transition state theory and the Rice-Ramsperger-Kassel-Marcus (RRKM) theory. Since both theories have classical dynamics at their foundation, advances in our understanding of nonlinear dynamics and continuing efforts to characterize the phase space structure of systems with three or more degrees of freedom are beginning to yield crucial mechanistic insights into the dynamics. This talk focuses on a mechanistic understanding of the deviations from RRKM theory for a model isomerization problem with three degrees of freedom. Several studies have established that such systems are prime candidates for observing non-RRKM behavior. The model is inspired, and generalized, from a much earlier study by De Leon and Berne. We try to answer two of the questions posed in this early work by studying the intramolecular vibrational energy flow in the system from both classical and quantum viewpoints. Using a wavelet-based local frequency analysis it is possible to construct a useful representation of the classical phase space (Arnol’d web) highlighting the important dynamical structures. Insights into the dynamics originate from the various nonlinear resonances and phase space traps which potentially result in quantum eigenstates of varying degree of localization.


Thursday, March 19, 2009 8:00AM - 10:48AM –
Session V39 DBP: Biological Networks and Systems Biology

8:00AM V39.00001 Boolean modeling of collective effects in complex networks1. JOHANNES NORRELL, JOSHUA SOCOLAR, Duke University Physics Department — Complex systems are often modeled as Boolean networks in attempts to capture their logical structure and reveal its dynamical consequences. Approximating the dynamics of continuous variables by discrete values and Boolean logic gates may, however, introduce dynamical possibilities that are not accessible to the original system. We show that large random networks of variables coupled through continuous transfer functions often fail to exhibit the complex dynamics of corresponding Boolean models in the disordered (chaotic) regime, even when each individual function appears to be a good candidate for Boolean idealization. A simple criterion identifies continuous systems that exhibit the full dynamical range of their Boolean counterparts. Transfer functions inferred from the literature on transcriptional regulation of genes do not satisfy the criterion.

1. This work was supported by grants from NSF (PHY-0417372) and NIH (1P50-GM081883).

8:12AM V39.00002 A Network Model For Sea Urchin Development1. XINWEI GONG, Department of Physics, Duke University, XIANRUI CHENG, Computational Biology and Bioinformatics Program, Duke University, JOSHUA SOCOLAR, Department of Physics, Duke University — The sea urchin embryo developmental gene regulatory network has been a subject of experimental study for decades. While current knowledge of the network is incomplete, boolean network models with autonomous updating can reveal dynamical features of the known network. Our analysis of such a model based on the network provided by Davidson et al [http://surg.caltech.edu/endomes/index.html] shows that, with the suggested initial inputs and certain sets of logic functions that are consistent with the known regulatory relations, a 3-cell system settles into an attractor that corresponds to the 3 different cell fates expected for the organism. The attractor is not sensitive to modest variations in the time delay parameters.

1. This research is supported by NSF and NIH through Grant Nos. PHY-0417372 and 1P50-GM081883.
8:24AM V39.00003 Achieving optimal growth: lessons from simple metabolic modules. SID-HARTRA GOYAL, Physics, THOMAS CHEN, Applied Mathematics, NED WINGREEN, Molecular Biology, Princeton University — Metabolism is a universal property of living organisms. While the metabolic network itself has been well characterized, the logic of its regulation remains largely mysterious. Recent work has shown that growth rates of microorganisms, including the bacterium Escherichia coli, correlate well with optimal growth rates predicted by flux-balance analysis (FBA), a constraint-based computational method. How difficult is it for cells to achieve optimal growth? Our analysis of representative metabolic modules drawn from real metabolism shows that, in all cases, simple feedback inhibition allows only optimal growth. Indeed, product-feedback inhibition is found in every biosynthetic pathway and constitutes about 80% of metabolic regulation. However, we find that product-feedback systems designed to approach optimal growth necessarily produce large pool sizes of metabolites, with potentially detrimental effects on cells via toxicity and osmotic imbalance. Interestingly, the sizes of metabolite pools can be strongly restricted if the feedback inhibition is ultraspesensitive (i.e. with high Hill coefficient). The need for ultraspesensitive mechanisms to limit pool sizes may therefore explain some of the ubiquitous, puzzling complexity found in metabolic feedback regulation at both the transcriptional and post-transcriptional levels.

8:36AM V39.00004 Bifurcation in stochastic differential equations with delayed feedback. GAUDREAU-L MATHIEU, JORGE VINALS, McGill University — The bifurcation diagram of a model nonlinear Langevin equation with delayed feedback is obtained numerically. This model relates to a common motif in genetic regulatory networks, and we study the effect of fluctuating parameters on the bifurcation diagram of the network. We observe both direct and oscillatory bifurcations in different ranges of model parameters. Below threshold, the stationary distribution function \( p(x) \) is a delta function at the trivial state \( x = 0 \). Above threshold, \( p(x) \sim x^\alpha \) at small \( x \), with \( \alpha = -1 \) at threshold, and monotonously increasing with the value of the control parameter above threshold. Unlike the case without delayed feedback, the bifurcation threshold is shifted by fluctuations by an amount that scales linearly with the noise intensity. With numerical information about time delayed correlations, we derive an analytic expression for \( p(x) \) which is in good agreement with the numerical results.

8:48AM V39.00005 Constraints imposed by nonfunctional protein-protein interactions on gene expression and proteome size. JINGSHAN ZHANG, Harvard University, SERGEI MASLOV, Brookhaven National Laboratory, EUGENE SHANKOVICH, Harvard University — Crowded intracellular environments present a challenge for proteins to form functional specific complexes while reducing nonfunctional interactions with promiscuous nonfunctional partners. Here we show how nonfunctional interactions limit the proteome diversity and the average concentration of co-expressed and co-localized proteins. We use yeast proteomes to verify our hypothesis that the proteome has evolved to operate closely to the upper limit of its size, while keeping individual protein concentrations sufficiently low to reduce nonfunctional interactions. These findings have implication for conceptual understanding of intracellular compartmentalization, multicellularity, and differentiation.

9:00AM V39.00006 Effect of TNF autocrine signaling on dosage-dependent NF-kappaB response to lipopolysaccharide stimulation. JAEWOOK JOO, BRYAN CARSON, CATHY BRANDA, JENS POSCHET, Sandia National Labs — We will present the dosage-dependent characteristics of NF-kappaB translocation patterns from single macrophages stimulated by E. Coli lipopolysaccharide. The NF-kappaB translocation patterns in single cells are found to be quite heterogeneous: The patterns are more heterogeneous with low dosage stimulation than with high dosage stimulation. For low dosage stimulation, most of cells take a rising pattern and we demonstrate that it is due to the TNFanalptra autocrine signaling effect. The above results are predicted and explained by a computational model, and corroborated and verified by a single cell fluorescence imaging technique.

9:12AM V39.00007 Gain control in molecular signaling without feedback1. ILYA NEMENMAN, Los Alamos National Laboratory — Statistical properties of environments experienced by biological systems in the real world change, and this requires adaptation to achieve a high fidelity information transmission in cellular networks. One form of such adaptive response is gain control. When the mean response of a signaling system is matched to the mean value of its signal, rescaling the gain allows to respond to signals with different variances without saturation and by utilizing the entire available dynamic range of the response. Here we argue that a certain simple mechanism of gain control, understood well in the context of systems neuroscience, translates to molecular signaling systems as well. The mechanism allows to transmit more than one bit (on or off) of information about the signal independently of the source variance. The mechanism does not require additional molecular circuitry beyond that already present in many molecular systems, and, in particular, it does not depend on existence of feedback loops. This analysis provides a plausible explanation for certain structural aspects of cellular networks.

9:24AM V39.00008 Noise in Random Boolean Networks. TIAO PEIXOTO, BARBARA DROSSEL, Technische Universität Darmstadt — We investigate the effect of noise on Random Boolean Networks. Noise is implemented as a probability \( p \) that a node does not obey its deterministic update rule. We define two order parameters, the long-time average of the Hamming distance between a network with and without noise, and its deterministic update rule. The bifurcation diagram of a model nonlinear Langevin equation with delayed feedback is obtained numerically. This model relates to a common motif in genetic regulatory networks, and we study the effect of fluctuating parameters on the bifurcation diagram of the network. We observe both direct and oscillatory bifurcations in different ranges of model parameters. Below threshold, the stationary distribution function \( p(x) \) is a delta function at the trivial state \( x = 0 \). Above threshold, \( p(x) \sim x^\alpha \) at small \( x \), with \( \alpha = -1 \) at threshold, and monotonously increasing with the value of the control parameter above threshold. Unlike the case without delayed feedback, the bifurcation threshold is shifted by fluctuations by an amount that scales linearly with the noise intensity. With numerical information about time delayed correlations, we derive an analytic expression for \( p(x) \) which is in good agreement with the numerical results.

9:36AM V39.00009 The effect of negative autoregulation on eukaryotic gene expression. DMITRY NEVOZHAY, RHYS ADAMS, Dept. of Systems Biology, UT M. D. Anderson Cancer Center, KEVIN MURPHY, Harvard Medical School, KRESIMIR JOSIC, Dept. of Mathematics, University of Houston, GÁBOR BALÁZSI, Dept. of Systems Biology, UT M. D. Anderson Cancer Center — Negative autoregulation is a frequent motif in gene regulatory networks, which has been studied extensively in prokaryotes. Nevertheless, some effects of negative feedback on gene expression in eukaryotic transcriptional networks remain unknown. We studied how the strength of negative feedback regulation affects the characteristics of gene expression in yeast cells carrying synthetic transcriptional cascades. We observed a drastic reduction of gene expression noise and a change in the shape of the dose-response curve. We explained these experimentally observed effects by stochastic simulations and a simple set of algebraic equations.

9:48AM V39.00010 Cell stimulation with optically manipulated microsources. HOLGER KRESS, JINGYU PARK, CECILE MEJEAN, JASON FORSTER, JASON PARK, SPENCER WALSE, DIANQING WU, Yale University, ORION WEINER, UC San Francisco, TAREK FAHYMI, ERIC DUFRESNE, Yale University — Many cells can sense spatial and temporal heterogeneities in concentrations of soluble molecules. The cellular signal transduction which forms the basis of this ability consists of signaling cascades and loops whose length and time scales are largely unknown. The systematic study of these networks requires control over the chemical microenvironment of cells. We present a novel technique to create molecular concentration patterns that are chemically, spatially and temporally flexible. Our approach uses optically manipulated colloidal particles which act as microsources of soluble molecules. This technique for flexible cell stimulation is combined with quantitative live cell microscopy measurements of cellular responses. We demonstrate the method by inducing chemotaxis in neutrophils. We quantify the intracellular calcium release, actin distribution, shape and motility of single cells. The possibility for quantitative stimulus-response measurements on single cells makes this method applicable to a wide range of systems biology studies.

1 Supported by DOE under Contract No. DE-AC52-06NA25586
10:12AM V39.00012 Determining Regulatory Networks Governing the Differentiation of Embryonic Stem Cells to Pancreatic Lineage. IPSITA BANERJEE, University of Pittsburgh — Knowledge of pathways governing cellular differentiation to specific phenotype will enable generation of desired cell fates by careful alteration of the governing network by adequate manipulation of the cellular environment. With this aim, we have developed a novel method to reconstruct the underlying regulatory architecture of a differentiating cell population from discrete temporal gene expression data. We utilize an inherent feature of biological networks, that of sparsity, in formulating the network reconstruction problem as a bi-level mixed-integer programming problem. The formulation optimizes the network topology at the upper level and the network connectivity strength at the lower level. The method is first validated by in-silico data, before applying it to the complex system of embryonic stem (ES) cell differentiation. This formulation enables efficient identification of the underlying network topology which could accurately predict steps necessary for directing differentiation to subsequent stages. Concurrent experimental verification demonstrated excellent agreement with model prediction.

10:24AM V39.00013 Stabilizing Motifs in Autonomous Boolean Networks and the Yeast Cell Cycle Oscillator¹. VOLKAN SEVIM, XINWEI GONG, JOSHUA SOCOLAR, Physics Department, Center for Nonlinear and Complex Systems, and IGSP Center for Systems Biology, Duke University, Durham, North Carolina 27708, USA — Synchronously updated Boolean networks are widely used to model gene regulation. Some properties of these model networks are known to be artifacts of the clocking in the update scheme. Autonomous updating is a less artificial scheme that allows one to introduce small timing perturbations and study stability of the attractors. We argue that the stabilization of a limit cycle in an autonomous Boolean network requires a combination of motifs such as feed-forward loops and auto-repressive links that can correct small fluctuations in the timing of switching events. A recently published model of the transcriptional cell-cycle oscillator in yeast contains the motifs necessary for stability under autonomous updating [1].


¹This research is supported by NSF and NIH through Grant Nos. PHY-0417372 and 1P50-GM081883.

10:36AM V39.00014 The Transition Pathway from Nonspecific to Specific Complex of DNA with a DNA-Bending Protein. SERGEI KUZNETSOV, PAULA VIVAS, YOGAMBIGAI VELMURUGU, ANJUM ANSARI, University of Illinois at Chicago — Integration host factor (IHF) from E. coli is a DNA-bending protein that recognizes and binds to its specific sites primarily by the indirect read-out mechanism, in which sequence-dependent DNA dynamics and flexibility play an important role. The crystal structure of IHF bound to a 35-bp long cognate site H indicates that the DNA is kinked at two sites separated by ~9 bp, resulting in a “U-turn” bend of the DNA. To probe the DNA bending dynamics, we use a laser T-jump, and time-resolved FRET on end-labeled DNA substrates. Our results show that DNA bending occurs on the same time-scales as thermal disruption of single base-pairs in B-DNA, suggesting that spontaneous kinking may be the rate-limiting step. To test this hypothesis, we modified the DNA at the site of the kinks by introducing (i) a nick in the sugar-phosphate backbone, and (ii) mismatches to create internal loops. For each of these substrates, the 4-20 fold increase in the binding affinity is reflected in a corresponding increase in the bending rates. Furthermore, the DNA bending rates are independent of the salt concentration. These results indicate that in the transition state ensemble the DNA is kinked, but specific protein-DNA interactions involving ion release have not occurred.

Thursday, March 19, 2009 8:00AM - 10:48AM
Session V40 DBP: Mechanics of Biomolecular Systems II

8:00AM V40.00001 Non-monotonic wave dispersion in one-dimensional spiral track of cardiac cells. TAE YUN KIM, OKYU KWON, KYOUNG J. LEE, Center for Cell Dynamics and Department of Physics, Korea University — Alternans, periodic cardiac beat-to-beat alternation, is an important precursor to cardiac fibrillation. The underlying mechanism for this phenomenon has been discussed mostly based on the electro-chemical kinetics of constituent cells (myocytes) that comprise the heart system. An important unexplored aspect of this phenomenon is the role of wave dispersion that reflects the cell-to-cell coupling as well as the local kinetic properties. A recent modeling study in fact suggests that a non-monotonic wave dispersion can be a source for alternans. We have designed and built very long (~ 15 cm) in vitro quasi-one dimensional tracks of rat ventricular cells for elucidating the instability responsible for the transition to alternans. One dimensional tracks are favorable, since it excludes the effect of local wave curvature. Systematic investigations based on S1-S2 stimulation protocols are carried out and here we present some preliminary evidence of non-monotonicity in cardiac wave dispersion.

8:12AM V40.00002 Periodic reversals allow bacteria to swarm. YILIN WU, University of Notre Dame, DALE KAISER, Stanford University, YI JIANG, Los Alamos National Laboratory, MARK ALBER, University of Notre Dame — Many bacteria can rapidly traverse surfaces from which they are extracting nutrient for growth. They generate flat, spreading colonies, called swarms because they resemble swarms of insects. We seek to understand how members of any dense swarm track their neighbors while interfering minimally with the motion of others’. We choose myxobacteria as our model system. Individual myxobacteria cells regularly reverse their gliding directions. With a cell- and behavior-based computational model, we show that reversals of gliding direction are essential for swarming and that reversals increase the outflow of cells across the edge of the swarm. We also find that the reversal period predicted to maximize the outflow of cells is the same (within the errors of measurement) as the period observed in experiments with normal myxobacteria cells. This coincidence suggests that the circuit regulating reversals evolved to its current sensitivity under selection for growth achieved by swarming. Our work suggests a crucial component in the general behavioral algorithm governing bacterial swarming.

8:24AM V40.00003 Do Recurred Sensory Organs in Drosophila Form Through a Turing-Type Bifurcation? YUHUIFENG ZHU, Department of Physics University of Houston — We study the recurved bristles on Drosophila wing margin of wild-type and mutant. The expression levels of the achase-caste complex protein determine the epidermal or neural fate of a pro-neural cell. In wide-type flies, the development ends in a state where a recurved bristle grows out nearly every fifth cell. Recent experiments have shown that the frequency of recurved bristles can be changed by adjusting the mean concentrations of the zinc-finger transcription factor Senseless and the micro-RNA miR-9a. With reduced levels of miR-9a, mutant flies grow regular organization of recurved bristles, but with a lower periodicity. We argue that the characteristics of bristle organization are signatures of a Turing-type bifurcation which emerges from a uniform background in reaction-diffusion process, in continua. In contract, fly wing margin consists of a discrete array of cells with possible cross-species interactions. Further, proteins do not diffuse between cells. We argue that the intracellular actions can play the role of diffusion in a discrete cell array. However, the analogs of diffusion coefficients can be positive or negative. Intracellular actions should give a conserved cell number periodicity. We introduce a simple model to study pattern formation in such cellular arrays based on intracellular actions. Also, we observe that periodicity both in length and cell numbers from different group of flies.
8:36AM V40.00004 Sisyphus at the Nanoscale: Bacterial Topotaxis in a Microfabricated Environment.  
GUILLAUME LAMBERT, Princeton University, PETER GALAUDTA, TU Deft, DAVID LIAO, ROBERT H. AUSTIN, Princeton University — The ballistic-like motion of self-propelled particles at low-Reynolds number can be exploited to influence their direction of motion. In particular, it has been demonstrated that by using the right topography (in this case a micro-fabricated array of funnel-like asymmetrical barriers), E.coli bacteria can be “pumped” between two adjacent regions (Galauda 2007, Wan 2008). We built upon this idea and developed a micro-habitat array in which chemotaxis and topotaxis—nutrient- and topology-driven movement, respectively—are in opposition, leading to an inherently unstable environment in which a bacterium is constantly pushed away from the fitness landscape’s summit in a Sisyphean fashion. Surprisingly, we find that the bacterial population as a whole is able to overcome the rectifying array. An in-depth microscopic analysis of the swimmer’s motion is used to quantify the strategies adopted by the bacteria.

1Partially supported by and performance at the CNF ECS-0335765, NBTC ECS-9876771, DARPA, NSERC, and NDSEG

8:48AM V40.00005 Microrheology of swimming bacteria suspension.  
ANDREY SOKOLOV, IGOR ARONSON, Argonne National Laboratory — We study rheology of suspension of swimming bacteria Bacillus Subtilis at high concentrations. Experiments were performed in a free standing fluid film contained in a transparent chamber with adjustable Oxygen/Nitrogen ratio. The swimming velocity of bacteria is controlled by the concentration of dissolved Oxygen: it reduces to zero when Oxygen is completely replaced by Nitrogen. Macroscopic flow in a film is produced by oscillations and rotations of magnetic particles by rotating external magnetic field. To extract the effective viscosity, we measured macroscopic velocity field generated by the particles using PIV of fluorescent markers seeded to the film. We discovered that viscosity of bacterial suspension is increasing with decreasing swimming speed of bacteria due lack of Oxygen.

This work was supported by the US DOE, grant DE-AC02-06CH11357.

9:00AM V40.00006 Microrheology of Actin Network Depends on Probe Size, Surface Chemistry and Depletion Effect.  
JUN HE, JAY TANG, Brown University — Microrheological properties of F-actin were measured by video particle tracking using beads with different size and surface chemistry. We found that the mean square displacements of probe particles scale with bead diameter with an exponent of about -0.45 instead of -1. This scaling behavior results in the measured shear moduli of F-actin network varying with the probe size. The main features of our data can be accounted for by the probe surface stickiness and the opposing depletion effect, both of which are confirmed by confocal imaging of beads in the actin network.

9:12AM V40.00007 Mechanics of biomimetic systems propelled by actin comet tails.  
HYERAN KANG, Department of Physics, Brown University, DHANANJAY TAMBE, School of Public Health, Harvard University, VIVEK SHENOY, Division of Engineering, Brown University, JAY TANG, Department of Physics, Brown University — The motility of intracellular bacterial pathogens such as Listeria monocytogenes is driven by filamentous actin comet tails in a variety of trajectories. Here, we present the in vitro study on the actin-based movements using spherical beads of different sizes coated with VCA protein, a partial domain of N-Wasp, in platelet extracts. Long term two-dimensional trajectories of the spherical beads motility show characteristic difference than those observed for bacteria, which have both elongated shape and asymmetric expression of the polymerization inducing enzyme. The trajectories also vary sensitively with the bead size and shape. These results provide a useful test to our new analytical model including the rotation of the bead relative to the tail.

TIMOTHY LEZON, ERAN EYAL, IVET BAHAR, University of Pittsburgh — Elastic network models (ENMs) are widely employed for approximating the coarse-grained equilibrium dynamics of proteins using only a few parameters. An area of current focus is improving the predictive accuracy of ENMs by fine-tuning their force constants to fit specific systems. Here we introduce a set of general rules for assigning ENM force constants to residue pairs. Using a novel method, we construct ENMs that optimally reproduce experimental residue covariances from NMR models of 68 proteins. We analyze the optimal interactions in terms of amino acid type, pair distances and local protein structures to identify key factors in determining the effective spring constants. When applied to several unrelated globular proteins, our method shows an improved correlation with experiment over a standard ENM. We discuss the physical interpretation of our findings as well as its implications in the fields of protein folding and dynamics.

9:36AM V40.00009 Pulling helices inside bacteria: imperfect helices and rings.  
ANDREW RUTENBERG, Dalhousie University, JUN ALLARD, University of British Columbia — We study steady-state configurations of intrinsically-straight elastic filaments constrained within rod-shaped bacteria that have applied forces distributed along their length. Perfect steady-state helices result from axial or azimuthal forces applied at filament ends, however azimuthal forces are required for the small pitches observed for MreB filaments within bacteria. Helix-like configurations can result from distributed forces, including co-existence between rings and imperfect helices. Levels of expression and/or bundling of the polymeric protein could mediate this co-existence.

9:48AM V40.00010 Bending rigidity of type I collagen homotrimer fibrils.  
SEJIN HAN, University of Maryland, SERGEY LEIKIN, National Institutes of Health, WOLFGANG LOSERT, University of Maryland — Normal type I collagen is an α1(I)/α2(I) heterotrimeric triple helix, but α1(I) homotrimers are also found in fetal tissues and various pathological conditions, e.g., causing bone fragility and reducing tendon tensile strength. It remains unclear whether homotrimers alter mechanical properties of individual fibrils or affect tissues by altering their organization at a higher level. To address this question, we investigated how homotrimers affect fibril bending rigidity. Homotrimer fibrils have been shown to be more loosely packed so that we expected them to be more susceptible to bending. However, homotrimer fibrils were more rigid despite being thinner and more hydrated. To quantify fibril rigidity, we analyzed their shape by Fourier decomposition, determined the correlation function for the direction along each fibril, and calculated the distribution of local fibril curvature. The estimated persistence length of homotrimer fibrils was 3 ~ 10 times longer than for heterotrimer fibrils, indicating much higher bending rigidity of homotrimer fibrils.

10:00AM V40.00011 Surface manipulation of protein filaments.  
LAURENT KREPLAK, DOUGLAS STAPLE, Dalhousie University, MARKO LOPARIC, Biozentrum, University of Basel, HANS-JUERGEN KREUZER, Dalhousie University — Within mammalian tissues, cells move by actively remodeling the structure of collagen fibrils. In order to study this situation, we analyze the force response of two types of filamentous protein structures, desmin intermediate filaments 12 nm in diameter and collagen fibrils 80 nm in diameter. Both types of filaments were adsorbed at a solid-liquid interface and locally moved with an AFM tip at constant velocity against surface friction in the interfacial plane. In the case of collagen fibrils, that have an extensibility below 30% extension, we observed that microns long fibrils could be moved by the tip and deformed into shapes that could not be explain by the linear elastic theory for a stiff rod. In the case of desmin filaments that can be stretched up to 3.5 times their length, we observed local stretching of the filaments and discreet steps in the torsional force measured with the cantilever. In order to describe both types of filaments' behaviors, we described the protein filaments as a chain of beads of mass m linked together by a mass-less polymer linker. By solving the Newtonian equations of motions for the coupled beads in the presence of a point load and a viscous drag due to the surface-filament interactions we were able to reproduced our experimental data and extract information on friction.

This work was supported by grants from NSERC.
impurities, suggesting that these defects play an important role in supersolidity. We have now extended our elastic measurements to both bcc and hcp below 200 mK. It has the same dependence on temperature, frequency, amplitude and bundling, and extension of the constituent fibrin molecules. We develop constitutive models that integrate these quantitative observations and suggest that fibrin extensibility and elasticity are largely manifestations of protein unfolding.

These measurements, and comparisons to new torsional oscillator results, clarify the roles of quantum statistics and crystal structure in the behavior of solid helium. A novel 'cysteine shotgun' method of labeling the in situ proteome reveals differences in assembly or conformation of several abundant cytoskeletal proteins, including vimentin, filamin and myosin.

A.C. Clark, J.T. West, Pennsylvania State University — After a multitude of experimental and theoretical efforts over the past few years attempting to explain the microscopic origin of non-classical rotational inertia (NCRI) signals seen in torsional oscillator (TO) experiments, disorder has emerged as a crucial factor for determining the supersolid behavior. In an attempt to discover the type of disorder relevant to the NCRI effect we have performed TO experiments on solid 4He impurity to a screw dislocation in solid 4He. Monte Carlo simulations addressed the physics of vacancy-induced supersolidity in 4He, Phys. Rev. Lett. 99, 155301 (2007).

We find that certain types of edge and screw dislocations are superfluid while other remain insulating, depending on their orientation, Burgers vector and possible splitting of the core. The mechanism for superfluidity is provided by the strain near the core of the defect exceeding a threshold value. Superfluid dislocations can build a network of phase coherent tubes (the so-called Shevchenko state), which might lead to an observable mass decoupling in experiment. I will also look at the interactions between a Helium-3 impurity atom and a screw dislocation and make contact with recent experiments.


This research was supported by NSERC and the University of Alberta

Experiments performed in collaboration with A.C. Clark and M.H.W. Chan with support from NSF grant DMR 0706359.
Using x-ray synchrotron radiation, we have studied the nature of crystals of solid $^3$He at temperatures down to 50 mK. Measurements of peak intensities and lattice parameters do not show indications of the supersolid transition. Between 50 mK and 0.6K the relative change in the lattice parameters is less than $2 \times 10^{-5}$ and that in $\langle u^2 \rangle$ less than $4 \times 10^{-3}$. Scanning with a small (down to $10 \times 10 \mu m^2$) beam, we resolve a mosaic structure within these crystals consistent with numerous small angle grain boundaries. The mosaic shows significant motion even at temperatures far from melting. When grown in aerogel, solid $^3$He polycrystalline, with an hcp crystal structure (as in bulk) and a crystallite size of approximately 100 nm. In contrast to the expectation that the highly disordered solid will have a large supersolid fraction, torsional oscillator measurements show a behavior that is strikingly similar to high quality crystals grown from the superfluid phase. The low temperature supersolid fraction is only $\sim 3 \times 10^{-3}$ and the onset temperature is $\sim 100$ mK. Work done in collaboration with C.A. Burns, M.H.W. Chan, C.N. Koditwakku, L.B. Lurio, A. Said and J.T. West.

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Thursday, March 19, 2009 11:15AM - 2:15PM — Session W2 DCM P Q1: Progress in Understanding the Nature of the 5/2 Fractional Quantum Hall State  
Spirit of Pittsburgh Ballroom BC

11:15AM W2.00001 Finite-Layer Thickness Stabilizes the Pfaffian State for the 5/2 Fractional Quantum Hall Effect: Wave Function Overlap and Topological Degeneracy  
MICHAEL PETERSON, University of Maryland — The fractional quantum Hall effect (FQHE) in the second orbital Landau level at even-denominator filling factor $5/2$ remains mysterious and is currently motivating many scientists not only because of its connection to a possible implementation of a fault tolerant topological quantum computer (Das Sarma et al., PRL 94, 166802(2005)). In this work, we theoretically consider the effect of the quasi-two-dimensional nature of the experimental fractional quantum Hall systems on a number of FQHE states in the lowest three orbital Landau levels. Our primary result is that the finite width of the quasi-two-dimensional systems produce a physical environment sufficient to stabilize the Moore-Read Pfaffian state thought to describe the FQHE at filling factor $5/2$. This conclusion is based on exact calculations performed in the spherical and torus geometries, studying wave function overlap and ground state degeneracy. Furthermore, our results open the possibility of creating optimal experimental systems where the $5/2$ FQHE state would more likely be described by the Moore-Read Pfaffian. We also discuss the role of the three-body interaction Hamiltonian that produces the Moore-Read Pfaffian as an exact ground state and particle-hole symmetry in the FQHE at $5/2$. We acknowledge support from Microsoft Project Q. Work done in collaboration with Sankar Das Sarma, Thierry Jojoliceur, and Kwon Park.

11:51AM W2.00002 Understanding the 5/2 fractional quantum Hall effect without the Pfaffian wave function  
CSABA TOKE, Lancaster University — The fractional quantum Hall effect (FQHE) in the second Landau level has attracted attention, because the lowest Landau level theories do not straightforwardly generalize to these states, and several of the proposed models feature excitations with non-Abelian braiding statistics, with possible applications in topological quantum computing. In particular, the FQHE states at $\nu = 5/2$ and $7/2$, which have no lowest Landau level analogons, are usually understood in terms of the paired composite fermion model proposed by Moore and Read. I present an alternative understanding of the $5/2$ FQHE within the composite fermion theory. I argue that the residual interaction between composite fermions plays a crucial role in establishing incompressibility at $5/2$. The low-energy spectrum and the activation gap are estimated with the help of a perturbative procedure that incorporates inter-composite-fermion interactions. This approach is amenable to systematic improvement, and produces ground as well as excited states. It, however, does not relate to non-Abelian statistics in any obvious manner. The emergence of incompressibility due to inter-composite-fermion interactions is also observed other fractions in the second Landau level, notably at $\nu = 2 + 2/5$ and $2+3/8$.

12:27PM W2.00003 Density Matrix Renormalization Group Studies of Incompressible Fractional Quantum Hall States  
ADRIAN FEIGUIN, Microsoft Station Q — In this talk I introduce a powerful technique, the density-matrix renormalization group (DMRG), for studying ground and excited state properties of incompressible FQH states on the sphere. This method not only reproduces the numerical results obtained earlier in the exact diagonalization studies, but we are able to extend our understanding of the ground-state and low-lying excited state properties of these FQH states to substantially larger system sizes. We address a very important open problem in fractional quantum Hall physics, namely, if the half-filled second Landau level state can exhibit non-Abelian statistics. By studying large systems on the sphere, and extrapolating to the thermodynamic limit, we determine that the ground state for this filling fraction is fully polarized for shifts corresponding to both the Moore-Read Pfaffian state and its particle-hole conjugate (anti-Pfaffian). This result is found to be robust against small variations of the interaction, strongly supporting the argument favoring a non-Abelian state. We further extend the application of this technique to identify other incompressible Hall states in the second Landau level.

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1 In collaboration with A. Phillis, J. Parpia, B. Cowan and J. Saunders.

nu=8/3 and 5/2. These measurements suggest significant roles for quasiparticle spin in the competing quantum phases that emerge in the second Landau level.

While the collapse of the spin wave at fillings near nu=1 had been linked to loss of spin polarization due to formation of spin textures, the low-lying excitation modes seen in the N=1 level below nu=3 seem much more complex because a sharp spin wave does not recover for fractional quantum Hall states such as the 7/3 FQH gap is observed to be enhanced by an applied parallel magnetic field, the 5/2 gap is strongly suppressed, in spite of the two gaps being energetically comparable at zero parallel fields in our sample. This calls into question the prevailing theoretical belief that they should behave similarly if both are spin-polarized, and raises doubt as to whether or not the 5/2 state is indeed described by a spin-polarized Pfaffian Moore-Read wavefunction.

1:15AM W3.00001 Single-molecule Force Spectroscopy of Intercellular Adhesion in Cancer, DENIS WIRTZ, Department of Chemical and Biomolecular Engineering, Johns Hopkins University — The progress of several human cancers correlates with the loss of a-catenin from E-cadherin-rich intercellular junctions and loss of adhesion. However, the potential role of a-catenin in directly modulating the adhesive function of individual E-cadherin molecules in human cancer is unknown. Here we use single-molecule force spectroscopy to probe the tensile strength, lifetime, and interaction energy between live human parental breast cancer cells lacking a-catenin and these cells where a-catenin is re-expressed. We find that the tensile strength and lifetime of single E-cadherin bonds between parental cells are significantly lower over a wide range of loading rates. Statistical analysis of the force-displacement spectra reveals that single cadherin bonds between cancer cells feature an exceedingly low energy barrier against tensile forces and low molecular rigidity. These results suggest that the loss of a-catenin drastically reduces the adhesive force between individual cadherin pairs on adjoining cells, explain the global loss of cell adhesion in human breast cancer cells and show that the forced expression of a-catenin in cancer cells can restore both higher intercellular avidity and intermolecular E-cadherin affinity.

1:15AM W3.00002 Studying Cell Motility and Cell Mechanics with “Designer Cells”, BARTOSZ A. GRZYBOWSKI, Department of Chemical and Biological Engineering, Northwestern University — Micro/nanopatterning allows for the creation of cells of identical morphologies and with “designed” organization of the cytoskeleton. Analysis of such “Designer Cells” via high-resolution microscopy allows for studying the intracellular processes related to cytoskeletal dynamics and cancer invasiveness in quantitative detail. In addition, three-dimensional imaging can be used to reconstruct cell shapes and describe these shapes by mathematical functions - it is found that cells are constant-curvature surfaces corresponding to the minima of relatively simple energy functionals describing cell micromechanics. These and other results have implications for physical assays with which to diagnose the metastatic form of cancer.

1:27PM W3.00003 Nanostructured Substrates for Capturing Circulating Tumor Cells in Whole Blood, HSIAN-RONG TSENG, Department of Molecular & Medical Pharmacology, Crump Institute for Molecular Imaging, David Geffen School of Medicine, UCLA — Over the past decade, circulating tumor cells (CTCs) has become an emerging “biomarker” for detecting early-stage cancer metastasis, predicting patient prognosis, as well as monitoring disease progression and therapeutic outcomes. However, isolation of CTCs has been technically challenging due to the extremely low abundance (a few to hundreds per ml) of CTCs among a high number of hematologic cells (109 per mL) in the blood. Our joint research team at UCLA has developed a new cell capture technology for quantification of CTCs in whole blood samples. Similar to most of the existing approaches, epithelial cell adhesion molecule antibody (anti-EpCAM) was grafted onto the surfaces to distinguish CTCs from the surrounding hematologic cells. The uniqueness of our technology is the use of nanostructured surfaces, which facilitates local topographical interactions between CTCs and substrates at the very first cell/substrate contacting time point. We demonstrated the ability of these nanostructured substrates to capture CTCs in whole blood samples with significantly improved efficiency and selectivity. The successful demonstration of this cell capture technology using brain, breast and prostate cancer cell lines encouraged us to test this approach in clinical setting. We have been able to bond our first validation study with a commercialized technology based on the use of immunomagnetic nanoparticles. A group of clinically well-characterized prostate cancer patients at UCLA hospital have been recruited and tested in parallel by these two technologies.
1:03PM W3.00004 A portable circulating tumor cell capture microdevice. RAM H. DATAR, Department of Pathology, Miller School of Medicine of University of Miami — Sensitive detection of earliest metastatic spread of tumors in a minimally invasive and user-friendly manner will revolutionize the clinical management of cancer patients. The current methodologies for circulating tumor cell (CTC) capture and identification have significant limitations including time, cost, limited capture efficiency and lack of standardization. We have developed and optimized a novel parylene membrane filter-based portable microdevice for size-based isolation of CTC from human peripheral blood. Following characterization with a model system to study the recovery rate and enrichment factor, a comparison of the microdevice with the commercially available system using blood from cancer patients demonstrated superior recovery rate and the promise of clinical utility of the microdevice. The development of the microdevice and its potential clinical applicability will be discussed.

1:39PM W3.00005 Detection and Characterization of Circulating Tumor Cells. RICHARD BRUCE, Scripps-PARC Institute for Advanced Biomedical Sciences, Palo Alto Research Center — Circulating tumor cells (CTCs) occur in blood below the concentration of 1 cell in a hundred thousand white blood cells and can provide prognostic and diagnostic information about the underlying disease. While enumeration of CTCs has provided useful information on progression-free and overall survival, it does not provide guidance of treatment choice. Since CTCs are presumed to contain features of their metastatic tissue, the characterization of cancer markers on these cells could help selection of treatment. At such low concentrations, reliable location and identification of these cells represents a significant technical challenge. Automated digital microscopy (ADM) provides high levels of sensitivity, but the analysis time is prohibitively long for a clinical assay. Enrichment methods have been developed to reduce sample size but can result in cell loss. A major barrier in reliable enrichment stems from the biological heterogeneity of CTCs, exhibited in a wide range of genetic, biochemical, immunological and biological characteristics. We have developed an approach that uses fiber-optic array scanning technology (FAST) to detect CTCs. Here, laser-printing optics are used to excite 300,000 cells/sec, and fluorescence from immuno-labels is collected in an array of optical fibers that forms a wide collection aperture. The FAST cytometer can locate CTCs at a rate that is 500 times faster than an ADM with comparable sensitivity and improved specificity. With this high scan rate, no enrichment of CTCs is required. The target can be a cytoplasm protein with a very high expression level, which reduces sensitivity to CTC heterogeneity. We use this method to measure expression levels of multiple markers on CTCs to help predict effective cancer treatment.


11:15AM W4.00001 Magnetically driven spiral ferroelectrics with high transition temperature, TSUYOSHI KIMURA, Division of Materials Physics, Graduate School of Engineering Science, Osaka University — In the past few years, a new class of materials such as orthorhombic rare earth manganites RMnO$_3$, both types of magnetic states are ferroelectric. This competition has important implications for the dynamic magnetoelectric coupling between spin waves and polar phonons resulting in mixed electromagnon excitations. We will discuss microscopic mechanisms of the single-magnon and bi-magnon excitation by an electric field of light in multiferroic and magnetoelectric materials, focusing in particular on the recently observed electromagnon peaks in orthorhombic manganites and Kagome magnets carrying monopole and toroidal magnetic moments. I will show that optical studies can provide useful information about competing multiferroic states in frustrated magnets.

1 Financial support of FOM is gratefully acknowledged.

12:27PM W4.00003 Multiferroic domain wall and its relevance to magnetoelectric phenomena in ferroelectric helimagnets. YOSHINORI ONOSE, University of Tokyo — Recently, magnetically induced ferroelectricity and the giant magnetoelectric (ME) effect in helimagnets (HMs) have attracted much attention. In the ferroelectric HMs, the ferroelectric domain walls (DWs) may be driven by the DW of the magnetic field along $b$-axis induces the $P$-flop $P||c$ to $P||a$. The dielectric constant shows a large enhancement in the course of the $P$-flop. We have investigated the dielectric dispersion of the giant magneto-capacitance (GMC) effect and found that the GMC is attributable to the motion of the DW between $bc$ plane spin cycloid ($P||c$) and $ab$ plane spin cycloid ($P||a$) domains.

In collaboration with H. Murakawa, K. Kagawa, S. Ishiwata, Y. Kaneko, K. Ohgushi, M. Mochizuki, N. Furukawa, and Y. Tokura
Thomson (Lord Kelvin) first posed the problem: what kind of foam of equal-sized bubbles minimises area (or energy)?

Carfrae of the Arup Corporation, it makes a spectacular impression on those who enter. It provokes thoughts on aesthetics, order/disorder, optimisation, and beams that are arranged as in the Weaire-Phelan structure of an ideal foam, with an outer facing of transparent “cushions.” Brilliantly conceived by Tristram "Water Cube," constructed for the Beijing Olympics, is unusual in that its very structure has a physical significance. It consists of a massive framework of steel perhaps the best known quasicrystal pattern.

were not understood in the West until the 1970s. I will discuss some of the properties of Islamic quasicrystalline tilings, and their relation to the Penrose tiling, construct nearly-perfect quasicrystalline patterns. These patterns have remarkable properties; they do not repeat periodically, and have special symmetry—and creation of increasingly complex periodic girih patterns, and by the 15th century, the tessellation approach was combined with self-similar transformations to zigzagging lines, and drafted directly with a straightedge and a compass. I discuss our recent findings that, by 1200 A. D., a conceptual breakthrough occurred. This result paves the way for a variety of investigations and theoretical predictions now varying both the hole doping x and J2. Other issues in the area of multifractals will also be addressed in this presentation, including the prediction of ferroelectricity in the spin zigzag E-type AF state.

First, the composite of two fractals is not generally scale invariant and exhibits complex multifractal scaling in the small flawed, and that fractal analysis as an authentication tool yields inconsistent and unreliable results. This work has also led to two new results in fractal analysis following the recent discovery of a cache of disputed Pollock paintings. I will demonstrate that this hypothesis of “Fractal Expressivism” is fundamentally characterized as fractal, and that fractal analysis can be used to authenticate works of unknown origin. This academic issue has become of more general interest issues in the area of multiferroics will also be addressed in this presentation, including the prediction of ferroelectricity in the spin zigzag E-type AF state. 

1 This work was supported by the NSF grant DMR-0706020 and the Division of Materials Science and Engineering, U.S. DOE, under contract with UT-Battelle, LLC.

Thursday, March 19, 2009 11:15AM - 1:39PM
Session W5 FPS: Physics Meets Art 401/402

11:15AM W5.00001 Quasicrystals in Medieval Islamic Architecture , PETER LU, Harvard University — The conventional view holds that girih (geometric star-and-polygon) patterns in medieval Islamic architecture were conceived by their designers as a network of zigzagging lines, and drafted directly with a straightedge and a compass. I discuss our recent findings that, by 1200 A. D., a conceptual breakthrough occurred in which girih patterns were conceived as tessellations of a special set of equilateral polygons (girih tiles) decorated with lines. These girih tiles enabled the creation of increasingly complex periodic girih patterns, and by the 15th century, the tessellation approach was combined with self-similar transformations to construct nearly-perfect quasicrystalline patterns. These patterns have remarkable properties; they do not repeat periodically, and have special symmetry—and were not understood in the West until the 1970s. I will discuss some of the properties of Islamic quasicrystalline tilings, and their relation to the Penrose tiling, perhaps the best known quasicrystal pattern.

11:51AM W5.00002 The Story of the Water Cube, DENIS WEAIRE, TCD, Dublin — The National Aquatics Center or “Water Cube,” constructed for the Beijing Olympics, is unusual in that its very structure has a physical significance. It consists of a massive framework of steel beams that are arranged as in the Weaire-Phelan structure of an ideal foam, with an outer facing of transparent “cushions.” Brilliantly conceived by Tristram Carfrae of the Arup Corporation, it makes a spectacular impression on those who enter. It provokes thoughts on aesthetics, order/disorder, optimisation, and the frequent recurrence of bubbles/foams in our literary and artistic culture. The story of the Water Cube will start in the nineteenth century, when William Thomson (Lord Kelvin) first posed the problem: what kind of foam of equal-sized bubbles minimises area (or energy)?

12:27PM W5.00003 The Drip Paintings of Jackson Pollock: Are They Really fractal?, KATHERINE JONES-SMITH, Case Western Reserve University — It has been claimed the drip paintings of late Abstract Expressionist painter Jackson Pollock can be usefully characterized as fractal, and that fractal analysis can be used to authenticate works of unknown origin. This academic issue has become of more general interest following the recent discovery of a cache of disputed Pollock paintings. I will demonstrate that this hypothesis of “Fractal Expressionsim” is fundamentally flawed, and that fractal analysis as an authentication tool yields inconsistent and unreliable results. This work has also led to two new results in fractal analysis of more general scientific significance. First, the composite of two fractals is not generally scale invariant and exhibits complex multifractal scaling in the small distance asymptotic limit. Second the statistics of box-counting and related staircases provide a new way to characterize geometry and distinguish fractals from Euclidean objects.

1:03PM W5.00004 Learning from Monet: A Fundamentally New Approach to Image Analysis1, CHARLES M. FALCO, University of Arizona — The hands and minds of artists are intimately involved in the creative process, intrinsically making paintings complex images to analyze. In spite of this difficulty, several years ago the painter David Hockney and I identified optical evidence within a number of paintings that demonstrated artists as early as Jan van Eyck (c1425) used optical projections as aids for producing portions of their images. In the course of making those discoveries, Hockney and I developed new insights that are now being applied in a fundamentally new approach to image analysis. Very recent results from this new approach include identifying from Impressionist paintings by Monet, Pissarro, Renoir and others the precise locations the artists stood when making a number of their paintings. The specific deviations we find when accurately comparing these examples with photographs taken from the same locations provide us with key insights into what the artists’ visual skills informed them were the ways to represent these two-dimensional images of three-dimensional scenes to viewers. As will be discussed, these results also have implications for improving the representation of certain scientific data. Acknowledgment: I am grateful to David Hockney for the many invaluable insights into imaging gained from him in our collaboration.

1 This work supported by ARO grant W911NF0610359.

Thursday, March 19, 2009 11:15AM - 2:15PM
Session W6 GQI: Progress on Quantum Optics with Circuit Quantum Electrodynamics 406
et al. provides a complete description of the quantum state. We analyze the prepared states by mapping out the corresponding Wigner function, which is the phase-space equivalent to the density matrix and in the resonator [1]. Using a generalization of this scheme [2] we can now create arbitrary quantum states of the photon field with up to approximately 10 photons. In both proposals we borrow from inspiring quantum-optical tools and concepts, exploiting the good control over a superconducting phase qubit by using it to pump photons into a high-fidelity measurement may be achieved [2]. In this situation, i.e., in pure vacuum, we have resolved the renormalization of the qubit transition frequency - known as the Lamb shift - due to its non-resonant interaction with the cavity vacuum fluctuations [3].


1Work done in collaboration with Johannes Fink, Andreas Fragner, Alexandre Blais, Peter Leek and the ETH Quantum Device Team.

11:51AM W6.00002 Nonlinear response of the vacuum Rabi resonance, JENS KOCH, Yale University — On the level of single atoms and photons, the coupling between atoms and the electromagnetic field is typically very weak. By employing a cavity to confine the field, the strength of this interaction can be increased many orders of magnitude to a point where it dominates over any dissipative process. This strong-coupling regime of cavity quantum electrodynamics has been reached for real atoms in optical cavities, and for artificial atoms in circuit QED and quantum-dot systems. A signature of strong coupling is the splitting of the cavity transmission peak into a pair of resolvable peaks when a single resonant atom is placed inside the cavity – an effect known as vacuum Rabi splitting. The circuit QED architecture is ideally suited for going beyond this linear response effect. Here, we show that increasing the drive power results in two unique nonlinear features in the transmitted heterodyne signal: the supersplitting of each vacuum Rabi peak into a doublet, and the appearance of additional peaks with the characteristic √n spacing of the Jaynes-Cummings ladder. These constitute direct evidence for the coupling between the quantized microwave field and the anharmonic spectrum of a superconducting qubit acting as an artificial atom. Work done in collaboration with L.S. Bishop, J.M. Chow, A.A. Houck, M.H. Devoret, E. Thuneberg, S.M. Girvin, and R.J. Schoelkopf.

12:27PM W6.00003 Preparation of arbitrary quantum states in a microwave resonator, MAX HOFHEINZ, University of California, Santa Barbara — Two-level systems, or qubits, can be prepared in arbitrary quantum states with exquisite control, just using classical electrical signals. Achieving the same degree of control over harmonic resonators has remained elusive, due to their infinite number of equally spaced energy levels. Here we exploit the good control over a superconducting phase qubit by using it to pump photons into a high-Q coplanar waveguide resonator and, subsequently, to read out the resonator state. This scheme has previously allowed us to prepare and detect photon number states (Fock states) in the resonator [1]. Using a generalization of this scheme [2] we can now create arbitrary quantum states of the photon field with up to approximately 10 photons. We analyze the prepared states by mapping out the corresponding Wigner function, which is the phase-space equivalent to the density matrix and provides a complete description of the quantum state.

11:15AM W7.00001 Optimizing information flow in biological networks, WILLIAM BIALEK, Princeton University — The generation of physicists who turned to the phenomena of life in the 1930s realized that to understand these phenomena one would need to track not just the flow of energy (as in inanimate systems) but also the flow of information. It would take more than a decade before Shannon provided the tools to formalize this intuition, making precise the connection between entropy and information. Since Shannon, many investigators have explored the possibility that biological mechanisms are selected to maximize the efficiency with which information is transmitted or represented, subject to fundamental physical constraints.

I will survey these efforts, emphasizing that the same principles are being used in thinking about biological systems at very different levels of organization, from bacteria to brains. Although sometimes submerged under concerns about particular systems, the idea that information flow is optimized provides us with a candidate for a real theory of biological networks, rather than just a collection of parameterized models. I will try to explain why I think the time is right to focus on this grand theoretical goal, pointing to some key open problems and opportunities for connection to emerging experiments.

11:51AM W7.00002 Form, Function, and Information Processing in Stochastic Regulatory Networks, CHRIS WIGGINS, Department of Applied Physics and Applied Mathematics; Columbia University — The ability of a biological network to transduce signals, e.g., from chemical information about the abundance of small molecules into regulatory information about the rate of mRNA expression, is thwarted by numerous sources of noise. A great amount has been learned and conjectured in the last decade about the extent to which the form of a network — specified by the connectivity and sign of regulation — constrains or guides the networks function — the particular noisy input-output relation(s) the network is capable of executing. In parallel, a great amount of research has sought to elucidate the role of inescapable or ‘intrinsic’ noise arising from the finite copy number of the participating molecules, which sets physical limits on information processing in small cells. I’ll discuss how information theory may help illuminate these topics by providing a framework for quantifying function which does not rely on specifying the particular task to be performed a priori, as well as by providing a measure for the extent to which form follows function. En route I hope to show how stochastic chemical kinetics, modeled by the (linear) master equation describing the probability of copy counts for all reactants, benefits from the same spectral approaches fundamental to solving the (linear) diffusion equation.

12:27PM W7.00003 Decision boundaries for maximizing information transmission in neural circuits¹, TATYANA SHARPEE, The Salk Institute for Biological Studies — Everything we know about the world around us is represented in the nervous system in sequences of discrete electrical pulses termed spikes. One attractive theoretical idea, going back to 1950s, is that these representations are efficient in the sense of information theory. I will describe an approach for finding the optimal coupling strengths between different neurons that is based on a concept of a decision boundary [1]. In this framework, neural circuit responses are described by specifying for each neuron the decision boundary that separates multi-dimensional signals that elicit a spike in that neuron from those signals that do not elicit a spike. The shape and position of individual neurons’ boundaries determine the amount of mutual information that the neural circuit can transmit about the incoming signals. Correspondingly, the optimal configuration of the decision boundaries depends on the probability distribution of incoming signals. Signals typical of our natural sensory environment are known to be strongly correlated and to possess large-amplitude deviations that are often better described by an exponential rather than a Gaussian distribution. Considering exponentially distributed signals, we find that optimal decision boundaries of neurons are curved, and that they exhibit sharp discontinuities when decision boundaries of different neurons intersect. This, in turn, corresponds to non-zero coupling constants when these neural circuits are described using the pairwise maximum entropy models.

¹NIH/NIMH, Alfred P. Sloan Fellowship, Searle Foundation

1:03PM W7.00004 Information processing and signal integration in bacterial quorum sensing, PANKAJ MEHTA, Princeton University — Bacteria communicate with each other using secreted chemical signaling molecules called autoinducers (AIs) in a process known as quorum sensing. Quorum sensing enables bacteria to collectively regulate their behavior depending on the number and/or species of bacteria present. The quorum-sensing network of the marine-bacteria *Vibrio harveyi* consists of three AIs encoding distinct ecological information, each detected by its own histidine-kinase sensor protein. The sensor proteins all phosphorylate a common response regulator and transmit sensory information through a shared phosphorylase that regulates expression of downstream quorum-sensing genes. Despite detailed knowledge of the *Vibrio* quorum-sensing circuit, it is still unclear how and why bacteria integrate information from multiple input signals to coordinate collective behaviors. Here we develop a mathematical framework for analyzing signal integration based on Information Theory and use it to show that bacteria must tune the kinase activities of sensor proteins in order to transmit information from multiple inputs. This is demonstrated within a quantitative model that allows us to quantify how much *Vibrio’s* learn about individual inputs and explains experimentally measured input-output relations. Furthermore, we predicted and experimentally verified that bacteria manipulate the production rates of AIs in order to increase information transmission and argue that the quorum-sensing circuit is designed to coordinate a multi-cellular developmental program. Our results show that bacteria can successfully learn about multiple signals even when they are transmitted through a shared pathway and suggest that Information Theory may be a powerful tool for analyzing biological signaling networks.

1:39PM W7.00005 to be determined by you, BORIS SHRAIMAN, USCB — No abstract available.
11:51AM W8.00002 Novel Detector developments for the European XFEL. HEINZ GRAF, DESY-Hamburg — The source properties of the Novel XFEL to be built in Hamburg impose extremely demanding requirements for the X-ray detectors that will be used in the experiments. The high luminosity of European XFEL, with many more pulses per second as compared to the American and Japanese projects, is one of the strong points that for sure will be used to the advantage in the experiments. The time structure is however such that the pulses are not distributed uniformly in time but are delivered in bunch trains (with up to 3000 bunches in a train) of 0.6 msec followed by 99.4 msec with no beam. This means that up to 3000 images will have to be recorded during the bunch train of 0.6 msec. This can only be achieved by temporarily storing the images in the detector, and reading them out during the 99.4 msec intervals. Furthermore, for every pulse of less than a 100 fsec a complete image has to be recorded, one can not use photon counting (“all photons arrive at the same time”), and one has to use integrating detectors, that record the total deposited X-ray energy, but with sufficiently low noise, so that one is able to distinguish between 0, 1, 2, 3, ... photons. On top of this one also wants to be able to record up to 10^4 photons, meaning a true dynamic range of more than 10^4, which is far from trivial. I will show various experimental examples, illustrating the specific detector challenges that follow from the above requirements. I will also discuss one solution, currently under development, which is the Adaptive Gain Integration Pixel Detector (AGIPD) project (DESY, PSI, Uni-Bonn, Uni-Hamburg). This detector is based on a classical Hybrid pixel array detector with a dynamically switchable gain stage to cope with the dynamic range, and an analog pipeline to store the recorded images during the 0.6 msec bunch train. Two other projects, LPD, and DEPFET will also be mentioned briefly.

12:27PM W8.00003 Integrating Pixel Array Detector Development. 1. SOL GRUNER, Cornell University — X-ray experiments are very frequently detector limited at storage ring synchrotron radiation sources, and will be even more so at future x-ray free electron laser and energy recovery linac sources. Limitations most frequently arise from the inability of detectors to efficiently collect and process data at the rates at which the data can be generated. Two bump-bonded silicon pixel array detectors (PADs) are being developed at Cornell University that will greatly enhance data collection capabilities. In these PADs x-rays are converted to electrical signals in a pixilated layer of high resistivity silicon, each pixel of which is connected by a metal solder “bump” to a corresponding pixel in a CMOS silicon integrated circuit. Each CMOS pixel contains its own data handling and processing electronics. Since all pixels operate in parallel, the PAD is capable of handling extremely high data throughput. The PAD pixels feature integrating analog front-end electronics which allow extremely high instantaneous count-rates, yet sufficiently high signal-to-noise to be able to detect single x-ray photons. The first PAD is designed for coherent x-ray imaging experiments at the Linac Coherent Light Source (LCLS) at SLAC. This detector frames continuously at the LCLS rate of 120 Hz, where the data for each frame can arrive in femtoseconds. The second detector, a result of a collaboration with the Area Detector Systems Corporation, is designed for high throughput protein crystallography experiments. Both detectors are described, and test data is provided. The capabilities of the detectors suggest a variety of new applications, some of which will be discussed. 1Supported by DOE & NIH.

1:03PM W8.00004 CMOS Hybrid Pixel Detectors for Scientific, Industrial and Medical Applications. CHRISTIAN BROENNIMANN, DECTRIS Ltd — Crystallography is the principal technique for determining macromolecular structures at atomic resolution and uses advantageously the high intensity of 3rd generation synchrotron X-ray sources. Macromolecular crystallography experiments benefit from excellent beamline equipment, recent software advances and modern X-ray detectors. However, the latter do not take full advantage of the brightness of modern synchrotron sources. CMOS Hybrid pixel array detectors, originally developed for high energy physics experiments, meet these requirements. X-rays are recorded in single photon counting mode and data thus are stored digitally at the earliest possible stage. The lead role for several advantages over current detectors: No detector noise is added to the signal. Readout time is reduced to a few milliseconds. The counting rates are matched to beam intensities at protein crystallography beamlines at 3rd generation synchrotron. The detector is not sensitive to X-rays during readout; therefore no mechanical shutter is required. The detector has a very sharp point spread function (PSF) of one pixel, which allows better resolution of adjacent reflections. Low energy X-rays can be suppressed by the comparator At the Paul Scherrer Institute (PSI) in Switzerland the first and largest array based on this technology was constructed: The Pilatus 6M detector. The detector covers an area of 43.1 x 44.8 cm^2, has 6 million pixels and is read out noise free in 3.7 ms. Since June 2007 the detector is in routine operation at the beamline 6S of the Swiss Light Source (SLS). The company DETCRIS Ltd, has licensed the technology from PSI and is commercially offering the PILATUS detectors. Examples of the wide application range of the detectors will be shown.


11:15AM W9.00001 Depinning transition in failure of disordered materials. LAURENT PONSON, California Institute of Technology, Pasadena, US — Crack propagation is the fundamental process leading to material failure. However, its dynamics is far from being fully understood. In this work, we investigate both experimentally and theoretically the far-from-equilibrium propagation of a crack within a disordered brittle material. The variations of its growth velocity v with respect to the external driving force G are carefully measured on a brittle rock of average fracture energy (T). The crack dynamics is shown to display two regimes, well described by a sub-critical creep law v ∝ G^(μ−1) with μ ≃ 1 for G < G_c, at low velocities, and a critical behavior where v ∝ (G – G_c)^(θ) with θ ≃ 0.8 when G > G_c. We show that these variations, as well as the value of the exponents μ and θ, can be explained extending the continuum theory of Fracture Mechanics to inhomogeneous media. In particular, these two regimes are shown to be reminiscent of the dynamical critical transition underlying the failure of disordered brittle materials.

11:27AM W9.00002 Random Organization and Irreversibility at Plastic Depinning. CHARLES REICHARDT, CYNTHIA REICHARDT, Los Alamos National Laboratory — We provide evidence that plastic depinning falls into the same class of phenomena as the random organization which was recently studied for periodically driven particle systems by L. Corte et al. [Nature Phys. 4, 420 (2008)]. In the plastic flow system that we consider, the pinned regime corresponds to a quiescent state while the moving regime corresponds to a fluctuating state. Upon the sudden application of an external force, the system organizes into one of these two states and the time scale required to reach the final state diverges as a power law when approaching a nonequilibrium transition. We propose a simple experiment to test this transition in colloidal systems with random disorder and in superconducting vortex systems.

11:39AM W9.00003 Static Avalanche s in a Random Landscape. 1. A. ALAN MIDDLETON, Syracuse University, PIERRE LE DOUSSAL, KAY J. WIESE, CNRS-LPTENS — We study jumps or avalanches in a model of a d-dimensional elastic interface that is pinned by disorder and tied to a harmonic spring. The interface configuration is the most stable one, given the disorder and spring position: as the spring is moved, this most stable configuration undergoes discrete jumps or shocks. We carry out numerical simulations to study these shocks and find: (1) detailed qualitative and quantitative verification of the validity of the functional renormalization group analysis of such interfaces and (2) that the distribution of avalanche sizes is numerically consistent with our new calculation of the exact shape of the avalanche distribution, computed in an ε = 4 – d expansion. The results are quite similar to those seen for dynamic avalanches, where the drive pushes interface configurations between metastable (not globally stable) states. 1NSF DMR 0606424 and ANR 05-BLAN-0099-01
11:51AM W9.00004 A simple model for deformation in solids with universal predictions for stress-strain curves and slip avalanches  . KARIN, DAHMEN, Dept. of Physics, University of Illinois at Urbana Champaign, YEHUDA BEN-ZION, Earth Sciences, University of Southern California, JONATHAN UHL, KARIN DAHMEN COLLABORATION, YEHUDA BEN-ZION COLLABORATION — A basic model for deformation of solids with only one tuning parameter (weakening epsilon) is introduced. The model can reproduce observed stress-strain curves, acoustic emissions and related power spectra, event statistics, and geometrical properties of slip, with a continuous phase transition from brittle to ductile behavior. Exact universal predictions are extracted using mean field theory and renormalization group tools. The results agree with recent experimental observations and simulations of related models for dislocation dynamics, material damage, and earthquake statistics.

12:03PM W9.00005 Hysteresis loop area of the kinetic Ising model with next-nearest neighbor interaction , WILLIAM BAEZ, TRINANJAN DATTA, CHRISTIAN POPPELIERS, Augusta State University — We investigate the effects of the next-nearest neighbor interaction on the hysteresis loop area of the two-dimensional kinetic Ising model subject to a time dependent magnetic field. For the nearest neighbor model it is known that the loop area, $A(H_o, f)$, has a dispersion relationship given by $A(H_o, f) \propto H_o^{2/3} f^{1/3}$ in the low frequency limit, $f \rightarrow 0$, where $H_o$ is the external magnetic field amplitude. Using the Metropolis algorithm we explore the hysteresis dispersion in the low frequency limit for various external magnetic fields. We find that the hysteresis relationship changes, as compared to the nearest neighbor model, in the presence of next-nearest neighbor interaction.

12:15PM W9.00006 Decay of metastable states in the N-neighbor Ising model . RANJIT CHACKO, HARVEY GOULD, Clark University, W. KLEIN, Boston University — We study the decay of metastable states in the N-neighbor Ising model in which each spin equally interacts with all other spins. Previous work has shown that near the pseudospinodal in an Ising model with long-range interactions nucleation occurs when many clusters which span a correlation volume coalesce to form the nucleating droplet. By observing the decay of a metastable state in the N-neighbor Ising model we can study the effect of the pseudospinodal on nucleation in a model which does not possess a length scale. This study has implications for spin-crossover materials.

12:27PM W9.00007 Physical criteria for comparing length and time scales of coarsening models , BENJAMIN VOLLMAYR-LEE, Bucknell University — A variety of models have been introduced to study the dynamics of phase separation, ranging from sub-critical kinetic Ising models to phase-field models to Oono and Puri’s cell dynamical systems (CDS). These models have in common that at asymptotic late times the dynamics reduces to that of sharp interfaces driven by a surface tension. In practical terms, one is typically interested in simulating these models into the asymptotic late-time regime, but it is not clear how to compare the rates of approach to asymptopia. Additionally, while the sharp interface dynamics have a high degree of universality, it is not clear to what degree this applies to the sub-asymptotic dynamics. A scheme is presented to address these questions. Essentially, one first identifies the relevant parameters that determine the asymptotic dynamics and leading sub-asymptotic dynamics. From these, the appropriate dimensionless measures of effective convergence can be obtained. The technique will be illustrated by a comparison of CDH to the Cahn-Hilliard phase field model.

12:39PM W9.00008 Dynamics of Nucleation in the Ising model . SEUNGHWA RYU, Physics Department, Stanford University, WEI CAI, Mechanical Engineering Department, Stanford University — While several theories have been developed to describe the kinetics of first order phase transitions, the range of applicability of each theory is not fully understood due to uncertainties in experiments and numerical difficulties in rare event simulations. In this study, we compute the decay rate of meta-stable states of the Ising model to test the validity of several existing nucleation theories. We employ advanced sampling methods to compute the nucleation rate, which spans a range over ten orders of magnitude, as a function of temperature and external field. Investigation of the critical nuclei and the pre-exponential factor reveals that nucleation in the 2d Ising model is well described by the field-theoretic model of Langer (1969). However, discrepancies between theory and numerical results are observed in the 3d Ising model. This discrepancy points to the importance of the shape of the critical nuclei to the nucleation kinetics.

12:51PM W9.00009 Scaling of the Island Density, Size Distribution and Capture Numbers in 3D Nucleation and Growth 13. JOHN ROYSTON, JAQUEM AMAR, University of Toledo — The results of kinetic Monte Carlo (KMC) simulations of a model of the irreversible nucleation and growth of fractal islands in 3D are presented along with a comparison with rate-equation (RE) results and mean-field (MF) theory. In previous work for point-islands in 3D it was found that both the scaled island-size distribution (ISD) and capture-number distribution (CND) approach the MF prediction of a diverging ISD and size-independent CND in the limit of large $D/F$ (where $D$ is the monomer diffusion rate and $F$ is the deposition rate). In contrast, here we find that the divergence of the ISD with increasing $D/F$ is much weaker for the case of fractal islands while the scaled CND $C(s/S)$ (where $S$ is the average island size) is not constant but increases linearly with island size $s$. We also find that the exponent $\chi$ describing the dependence of the peak island-density on $D/F$ (e.g. $N_{pk} \sim (D/F)^{-\chi}$) deviates significantly from the standard prediction $\chi = 1/3$. Self-consistent RE results for the average island and monomer densities which give good agreement with simulations are also presented, along with an analytical expression for the exponent $\chi$.

1Supported by NSF DMR-0606307

1:03PM W9.00010 The effects of spatial symmetry breaking on unstable state evolution , RACHELE DOMINGUEZ, KIPTON BARROS, W. KLEIN, Boston University — We develop a theory that predicts two distinct stages for the early unstable kinetics of systems with spatial symmetry breaking transitions. In the first stage the kinetics is dominated by symmetry preserving dynamics which acts on a short time scale. In the second stage, which shares some characteristics with the Cahn-Hilliard-Cook theory, noise driven fluctuations break the symmetry of the initial phase on a time scale that is large compared to the first stage for systems with an effective long-range interaction. Our simulations of the initial evolution of a long-range antiferromagnetic Ising model quenched into an unstable region are consistent with our predictions.

1:15PM W9.00011 Liquid to solid nucleation through onion-structure droplets13 , KIPTON BARROS, WILLIAM KLEIN, Boston University — We start from a Landau-Ginzburg free energy and develop a theory of crystal nucleation for metastable liquids. Saddle points of the free energy represent nucleating droplets and are obtained analytically and numerically. We find nucleating droplets with hexagonal symmetry in two dimensions and bcc and icosahedral symmetries in three dimensions. Surprisingly, we also find nucleating droplets in three dimensions with a spherically symmetric structure resembling the layers of an onion. These onion-structure objects are the preferred nucleating droplets near the spinodal. We discuss recent experiments and simulations which are consistent with our predictions.

1This work was funded by DOE Grant No. 2234-5 and NSF Grant No. DGE-0221680.

13Funded in part by NSF Grant No. DGE-0221680 and DOE Grant No. 2234-5.
1:27PM W9.00012 Dynamical non-ergodic scaling in continuous finite-order quantum phase transitions, SHUHA DENG, GERARDO ORTIZ, LORENZA VIOLA, Dartmouth College — We investigate the emergence of universal dynamical scaling in quantum critical spin systems adiabatically driven out of equilibrium, with emphasis on quench dynamics which involves non-isolated critical points (i.e., critical regions) and cannot be a priori described through standard scaling arguments nor time-dependent perturbative approaches. Comparing to the case of an isolated quantum critical point, we find that non-equilibrium scaling behavior of a large class of physical observables may still be explained in terms of equilibrium critical exponents. However, the latter are in general non-trivially path-dependent, and detailed knowledge about the time-dependent excitation process becomes essential. In particular, we show how multiple level crossings within a gapless phase may completely suppress excitation depending on the control path. Our results typify non-ergodic scaling in continuous finite-order quantum phase transitions.

1:39PM W9.00013 A deposition model with temperature dependent diffusion, YEN-LIANG CHOU, MICHEL PLEIMLING, Virginia Polytechnic Institute and State University — We study a deposition process where the deposited particles are allowed to hope to their neighboring sites with a probability that depends both on the temperature and on the height difference. Changing the temperature, the model evolves from the random deposition model with surface relaxation at zero temperature to the random deposition model at infinite temperature. A generalized dynamic scaling of the surface width as a function of the lattice size, the deposition time, and the temperature is given. The response to a sudden change in temperature is studied. Two types of quenching behavior are observed: a power law decay within the Edwards-Wilkinson regime and an exponential decay in the saturation regime.

1:51PM W9.00014 Hydrodynamic limit of a model of unstable diffusive interface growth, MATTEO NICOLI, Universidad Carlos III de Madrid, MARIO CASTRO, Universidad Pontificia Comillas de Madrid, RODOLFO CUERNO, Universidad Carlos III de Madrid — Recently we have proposed a stochastic moving boundary model to describe the morphological evolution of a large class of diffusive growth systems, with thin film production by Chemical Vapor Deposition and Electrochemical Deposition (ECD) as relevant physical examples. The model has a direct connection with measurable experimental parameters. In order to study the hydrodynamic limit of this model we have performed a small slopes expansion (SSE) that leads to an effective interfacial stochastic equation (ISE). In case of attachment kinetics much larger than the mean growth velocity the kinetic roughening exponents of this ISE are completely different from those of standard universality classes. This equation is a particular instance of a new class of nonlocal interface equations whose novel properties we have studied by numerical and RG techniques. In order to study the model beyond the SSE we have mapped it into an equivalent phase-field model. Numerical simulations of the latter show a remarkable quantitative agreement with ECD experiments.

2:03PM W9.00015 The Isothermal Dendritic Growth Experiment Archive, MATTHEW KOSS, College of the Holy Cross — The growth of dendrites is governed by the interplay between two simple and familiar processes—the irreversible diffusion of energy, and the reversible work done in the formation of new surface area. To advance our understanding of these processes, NASA sponsored a project that flew on the Space Shuttle Columbia in 1994, 1996, and 1997 to record and analyze benchmark data in an apparent-microgravity “laboratory.” In this laboratory, energy transfer by gravity driven convection was essentially eliminated and one could test independently, for the first time, both components of dendritic growth theory. The analysis of this data shows that although the diffusion of energy can be properly accounted for, the results from interfacial physics appear to be in disagreement and alternate models should receive increased attention. Unfortunately, currently and for the foreseeable future, there is no access or financial support to develop and conduct additional experiments of this type. However, the benchmark data of 35mm photonegatives, video, and all supporting instrument data are now available at the IDGE Archive at the College of the Holy Cross. This data may still have considerable relevance to researchers working specifically with dendritic growth, and more generally those working in the synthesis, growth & processing of materials, multiscale computational modeling, pattern formation, and systems far from equilibrium.

3Work supported by NASA’s erstwhile Physical Science Research Division (Code UG)


11:15AM W10.00001 First-principles theory of coloration of WO₃ upon charge insertion, YU XUE, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, USA — Tungsten trioxide is one of the most extensively studied electrochromic materials. Here we report density functional theory (DFT) investigations of the coloration mechanism of WO₃ upon charge insertion. Our results explains very well the systematic change in color of Na₃WO₃ from blue to golden-yellow with increasing sodium concentration. We find that proper accounts for the free-carriers contribution to the optical response are critical for a quantitative understanding of the coloration mechanism in this system. We thank Dr. Yong Zhang for his helpful discussion. We thank Dr. M. D. Jones for his assistance in coding. We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY.

1This work was supported in part by National Science Foundation Grant No. CBET-0844720 and by the UB 2020 Interdisciplinary Research Development Fund (IRDF).

11:27AM W10.00002 First principles studies of Ce and Eu-doped inorganic, ANDREW CANNING, ANURAG CHAUDHRY, ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — This work presents the results of first principles electronic structure calculations for europium and Ce doped inorganic compounds performed using the pseudopotential method based on the local spin density approximation (LSDA) and generalized gradient approximation+U (GGA+U) in density functional theory. The positions of the europium and cerium 4f and 5d states relative to the valence band maximum and conduction band minimum of the host material are determined. Qualitative predictions of the brightness of scintillation in the doped material is made based on the following criteria: (1) The size of the host material bandgap (2) The energy difference between the VBM (Valence Band Maximum) of the host material and the dopant 4f level (3) The energy difference between the occupied Eu or Ce 5d excited state and the host material CBM (Conduction Band Minimum) (4) The level of localization of the 5d excited state on the dopant atom. We have validated this theoretical approach on examples of known bright scintillators and non-activated scintillators. We have performed calculations on new Eu doped compounds to determine if they are candidates for Eu²⁺ activated scintillators

2Research supported by the U.S. Department of Homeland Security

3Work supported provided by the Center for Computational Research at the University at Buffalo, SUNY.
Electronic structure of the quasi-two-dimensional spin-gap system SrCu$_2$(BO$_3$)$_2$, ANDRES SAUL, CINaM/CNRS (Marseille, France), GUILLAUME RADTKE, IM2NP (Marseille, France), H. DABKOWSKA, B. GAULIN, G. BOTTON, McMaster University (Ontario, Canada) — During the last decade, a lot of theoretical and experimental work has been devoted to the study of the magnetoelectric coupling in quasi-two-dimensional (Q2D) layered systems. One of the most studied of such systems is SrCu$_2$(BO$_3$)$_2$, which is known to exhibit a rich variety of magnetic and electronic properties due to the presence of spin distortions. This compound is a prototypical example of a spin-gap system, where the magnetic excitations are suppressed below a certain temperature, leading to a gap in the excitation spectrum. In this talk, we will present the results of our recent calculations aimed at understanding the electronic and magnetic properties of SrCu$_2$(BO$_3$)$_2$, with a particular focus on the role of interlayer coupling. We will discuss the implications of our findings for the understanding of the magnetoelectric coupling in this and related systems.

PDMS-BaTiO$_3$, Composite with Mechanically Tunable Optical Properties, NASSER MOHAMED, MOISES HINOJOSA, VIRGILIO GONZALEZ, FIME-UANL — Novel composites that show visible light transmittance, mechanically tunable refractive index and good mechanical properties based on PDMS and BaTiO$_3$ (BT) nanoparticles (NP), were prepared in 2 steps. First, the NPs were obtained via mechanical milling; the BT was used as-purchased. Average particle sizes of ∼100nm were selected. Second, the NP were embedded into PDMS by in-situ polymerization. PDMS from Dow Corning (Silgard 184) was supplied as a kit containing 2 components: the Base and the Curing Agent. The BT content was varied up to 1.0wt%. Finally, thick films were prepared by solvent casting and cured in a vacuum furnace, where the trapped air and solvent were extracted. Weight content of the NP was examined. XRD and Raman confirmed the desired tetragonal phase of BT NP. Average particle size was determined by SEM, EDS maps revealed a homogeneous dispersion of the NP. UP-VIS analysis showed transmittances of ∼70%. The ellipsometry results revealed that the wt% of BT significantly influences the optical response of the composite when it is stressed, however the response is not linear.

Measuring Quantum Efficiency of Organic Dyes Encapsulated in Dielectric NanoSpheres, TIMOTHY RUSSIN, Department of Physics, The Pennsylvania State University, ERHAN ALTINOGLU, JAMES ADAIR, Department of Materials Science and Engineering, The Pennsylvania State University, PETER EKULUND, Department of Physics, Department of Materials Science and Engineering, The Pennsylvania State University — We present results of a fluorescent quantum efficiency (Φ) study on the encapsulation of the near infrared dye indocyanine green (ICG) in calcium phosphate (CP) nanoparticles (dia~50 nm). The quantum efficiency (Φ, described as the ratio of photons emitted to photons absorbed) provides a quantitative means of describing the fluorescence of an arbitrary molecule. However, standard quantum efficiency measurement techniques provide only Φ of the smallest fluorescing unit — in the case of a nanoparticle suspension, the nanoparticle itself. This presents a problem in accurately describing the quantum efficiency of fluorophores embedded in a nanoparticle. We have developed a method to determine the quantum efficiency of a constituent molecule embedded in such a nanoparticle, which provides a more meaningful comparison with the unencapsulated fluorophore. While applicable to generic systems, we present results obtained by our method for the ICG/CP nanoparticles in phosphate buffer solution, revealing a dramatic improvement in per-molecule Φ driven by encapsulation.

Dynamic mean-field analysis of the photo-induced insulator-metal transition in correlated electron systems — pump-probe spectroscopy, NAOTO TSUJI, TAKASHI OKA, HIDEO AOKI, Department of Physics, University of Tokyo — Recent pump-probe spectroscopy experiments have revealed that photo-excitation can trigger a ‘phase transition’ from an insulator to a metal in various strongly correlated materials. The transition, occurring inherently out of equilibrium, is distinct from conventional phase transitions. In order to identify the nature of the states emerging during the irradiation of an intense laser, we employ the dynamical mean-field theory combined with the Floquet technique for ac fields, which enables us to take account of both the electron correlation and the nonlinear electric-field effect, two essential ingredients in the photo-induced phenomenon. We apply the method to the Falicov-Kimball model, one of the simplest models of correlated electrons, coupled to an ac pump light. The derived optical conductivity spectrum exhibits a Drude-like peak in the low-energy region indicative of metallization. We have also obtained the nonequilibrium distribution of electrons, which turns out to very much deviate from the Fermi distribution, so that the phenomenon is distinct from the heating effect picture. Interestingly, a dip structure is found to emerge in the charge transfer peak, which is shown to come from the vertex correction. We also discuss the dependence of the optical conductivity on the photon energy of the pump light.


Group IIIA doping in $\alpha$-Fe$_2$O$_3$ for PEC hydrogen production, MUHAMMAD N. HUDA, ARON WALSH, YANPA YAN, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO 80401; YONG-SHENG HU, ALAN KLEIMAN-SHWARSTEIN, ERIC MCFARLAND, Dept. of Chemical Engineering, University of California at Santa Barbara, CA 93106; MOWAFAK AL JASSIM, National Renewable Energy Laboratory, Golden, CO 80401 — Among iron oxides, $\alpha$-Fe$_2$O$_3$ is the most abundant on earth. Because it has a band gap of approximately 2 eV, it is stable and inexpensive to process, $\alpha$-Fe$_2$O$_3$ has been considered as a potential photoelectrocatalyst for solar driven photoelectrochemical (PEC) water splitting to make hydrogen. However, as $\alpha$-Fe$_2$O$_3$ is a charge-transfer type insulator, the poor conduction properties have limited its efficiency as a PEC material. We will present our study on the doping of group IIIA elements in $\alpha$-Fe$_2$O$_3$ to improve its performance. All the calculations were done with DFT+$U$. The main electronic features of $\alpha$-Fe$_2$O$_3$ remained almost unchanged for group IIIA doping. While for Al-doping, the band gap remained almost the same, for Ga and In substitution the band gap marginally increased. However, increased conduction and PEC efficiency has been experimentally reported for Al-doped $\alpha$-Fe$_2$O$_3$. It will be shown that the change in volume plays an important role in this behavior. A dramatic increase in photo-response cannot be expected for this type of doping in $\alpha$-Fe$_2$O$_3$.
12:51PM W10.00009 The band gap of ultra-thin amorphous and well-ordered Al$_2$O$_3$ films on CoAl(100)$^1$. VOLKER ROSE, Argonne National Laboratory, RENE FRANCHY$^2$. Research Center Julich — Understanding the insulating properties of thin oxide films is key to developing novel devices. In this work, the band gaps of ultra-thin amorphous and well-ordered alumina films on CoAl(100) were investigated by means of scanning tunneling spectroscopy (STS). The ordered intermetallic alloy CoNi(100) exhibits a magnetic surface, although the bulk is nonmagnetic. Such a material is extremely attractive for innovative technical applications. Utilizing selective oxidation, by which the oxidation of CoAl leads to surface segregation of the element with higher oxygen affinity, high-quality Al$_2$O$_3$ films are formed. Oxidation at 300 K leads to the growth of amorphous oxide, while well-ordered films result at elevated temperatures. In both cases, the self-limiting thickness of the oxide film amounts to around 1 nm. The analysis yields band gaps of 2.8 and 3.6 eV for amorphous and well-ordered Al$_2$O$_3$, respectively. The with respect to the bulk oxide reduced band gap can be explained by the appearance of defect induced states localized in the band gap.

$^1$This work was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

$^2$deceased

1:03PM W10.00010 Spectroscopic analysis of ALD-coated 3D structures and origin of the Berreman effect. GIOVANNA SCAREL, JEONG-SEOK NA, KEVIN HYDE, GREGORY PARSONS, North Carolina State University, PARSONS GROUP TEAM — The Berreman effect sheds light on various phenomena in 2D systems. However, coatings of 3D systems in soft-lithography and photonic devices, or 3D fibers suggest that the Berreman effect in 3D structures could be different. Experimental and computational infrared spectroscopy studies of 3D structures conformally coated with Al$_2$O$_3$ and ZnO layers using atomic layer deposition support this conclusion. In 2D systems, defining $\theta_0$ the macroscopic incidence angle of the IR beam on a sample, the LO mode absorbance increases as $|\sin(\theta_0)|^2$ when $\theta_0$ becomes grazing. On the other hand, in 3D systems a linear combination of $|\sin(\theta_0)|^2$ with appropriate coefficients must be considered. Accounting for Snell’s law in the simulation model is essential to explain these results and the origin of the Berreman effect. We conclude that sample geometry determines infrared absorbance of LO modes versus $\theta$ and vice-versa.

Our results promise a new tool to investigate topography of insulating ionic oxide layers.

1:15PM W10.00011 Dielectric properties of solids in the regular and split charge equilibration formalisms. RAZVAN NISTOR, MARTIN MÜSER, University of Western Ontario — We investigate the generic dielectric properties of solids in which atomic charges are assigned within the split-charge equilibration (SQE) method, which contains the regular charge equilibration method as a limiting case. It is shown that the latter always mimics ideal conductors, while any positive bond hardness, which is introduced in the SQE method, turns the solid into a dielectric. Crystals with simple cubic and rocksalt structure are considered explicitly. For these symmetries we map the split-charge formalism onto a continuum model, which can be solved analytically, e.g., we provide simple analytical expressions for how the dielectric constant and penetration depth depend on atomic hardness, bond hardness, and lattice constant. This mapping may prove useful when having to solve the dielectric response of a heterogeneous system to external electrical fields not only on the atomic but also on a coarse-grained scale. Successful comparison of numerical data to analytical solutions is made, including those that contain discretization corrections to the continuum solution.

1:27PM W10.00012 Charge and Bonding States of Ag Atoms in Superionic Conductor $\alpha$-AgI. MASATO ITO, KAZUO TSUMURAYA, Meiji University, Japan — The fast migration mechanism of the cations in the superionic conductors has been little known up to now. In the case of $\alpha$-AgI, the charge states of the Ag atoms and the bonding states between Ag and I atoms during the migration remain to be explained. No explanation has also been given for the origin of both the positions and the asymmetric first peaks of the Ag-I and Ag-Ag pair distribution functions. We investigate the electronic states of AgI using the first principles electronic structure calculations. We use the Bader analysis to evaluate the charges that belong to each atom and obtain the ionicity of the atoms. The stability of the cation pairs in the conductor will be discussed using their binding energies.

1:39PM W10.00013 Multiplets and Crystal Fields: Systematics for X-Ray Spectroscopies. FRANCOIS VERNAY, BERNARD DELLEY, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — Recently Soft X-ray spectroscopies such as XAS andRIXS, became tools of choice to investigate transition metal oxides. The current resolving power is such that it is nowadays possible to investigate multiparticle excitations like, for instance, bi-magnon dispersion throughout the entire Brillouin zone. Yet, these spectroscopies are strongly linked to local physics: the absorption of a photon and creation of a localized core-hole opens up a shell and therefore a multiplet structure becomes apparent in the spectra. From here we see that it becomes crucial, while interpreting the experimental data, to have a systematic, user-friendly and transparent way of computing the multiplet spectra in order to disentangle in the experiment the information arising from single-particle excitations from the information relevant to collective excitations. We present our approach for arbitrary core-valence multiplets arising from a single configuration. The method covers the full range LS-intermediate-jj and allows to introduce splitting by an arbitrary crystal field easily.

Thursday, March 19, 2009 11:15AM - 2:03PM –
Session W11 DMP: Focus Session: Transport Properties of Nanostructures VI: Kondo Phenomena

11:15AM W11.00001 Very high Kondo temperature ($T_K \sim 80$ K) in single self-assembled InAs quantum dots coupled to metallic nanogap electrodes. KENJI SHIBATA, KAZUHIKO HIRAKAWA, IIS and INQIE, University of Tokyo — We have studied electron tunneling through single self-assembled InAs quantum dots (QDs) laterally coupled to metallic nanogap electrodes. Lateral electron tunneling structures were fabricated by forming nanogap metallic electrodes directly upon single self-assembled InAs QDs grown on GaAs surfaces. The n-type substrate was used as a backgate electrode. Although no intentional tunneling barriers were introduced, the fabricated samples worked as single electron transistors and exhibited Coulomb blockade effect. Furthermore, a clear spin-half Kondo effect was observed when strong coupling between the electrodes and the QDs was realized using a large QD with a diameter of $\sim 100$ nm. From the temperature dependence of the linear conductance at the Kondo valley, the Kondo temperature, $T_K$, was determined to be $\sim 81$ K. This is the highest $T_K$ ever reported for artificial semiconductor nanostructures. This high Kondo temperature is due to strong QD-electrode coupling and large charging/orbital-quantization energies in our self-assembled InAs QD structures.

$^1$This work was partly supported by the JST (CREST), Grants-in-Aid from the JSPS (No.18201027 and No.19560338), the grant from the Mazda Foundation, and the Specially Coordinated Fund from MEXT.
11:27AM W11.00002 Reduced Kondo conductance in a quantum dot by a high-biased quantum point contact nearby

KENICHI HITACHI, Department of Physics, University of Tokyo, AKIRA OIWA, SEIGO TARUCHA, Department of Applied Physics, University of Tokyo — A quantum point contact (QPC) near a quantum dot (QD) can be used for detecting the charge state in a QD. Also a single spin in a QD can be monitored by pulsed gate operation. However it has been shown that applied QPC source-drain bias voltage induces undesirable charge and spin fluctuations in a QD, such as photon-assisted like tunneling in a Coulomb blockade regime or suppressing conductance at spin-half Kondo valley. In this experiment, we examined the influence of Kondo valley and inelastic cotunneling at Coulomb valley in detail. We found that decreasing conductance at Kondo valley can be explained by the increase of local temperature, which is estimated by the conductance at inelastic cotunneling. We predict that this local increase of temperature is caused by the back-action between a QD and a QPC. This gives an alternative explanation of suppressing conductance at Kondo valley, which was thought to be the effect of dephasing a spin singlet between the dot and the lead.

11:39AM W11.00003 A magnetic field-induced crossover to a non-universal regime in a Kondo dot

ANDREI KOGAN, TAI-MIN LIU, BRYAN HEMINGWAY, University of Cincinnati, STEVEN HERBERT, Xavier University, MICHAEL MELLOCH, Purdue University, UNIVERSITY OF CINCINNATI TEAM, XAVIER UNIVERSITY COLLABORATION, PURDUE UNIVERSITY COLLABORATION — We have measured the magnetic splitting, $\Delta_K$, of a Kondo peak in the differential conductance of a Single-Electron Transistor while tuning the Kondo temperature, $T_K$, along two different paths in the parameter space: varying the dot-lead coupling at a constant dot energy, and vice versa. At a high magnetic field, $B$, the changes of $\Delta_K$ with $T_K$ along both paths have opposite signs, suggesting that $\Delta_K$ is not a universal function of $T_K$. At low $B$, we observe a decrease in $\Delta_K$ with $T_K$ along both paths. Detailed $\Delta_K(B)$ data for two different $T_K$ show consistency for the splitting onset. Furthermore, we find $\Delta_K/\Delta < 1$ at low $B$ and $\Delta_K/\Delta > 1$ at high $B$, where $\Delta$ is the Zeeman energy of the bare spin. We discuss an approximate scaling of $\Delta_K$ with $B/T_K$ at low $B$ and compare the findings to previous measurements and theory.

$^3$The research is supported by NSF DMR award No. 0804199 and by University of Cincinnati.

11:51AM W11.00004 Correlated Wavefunction Description of Kondo States on Metal Surfaces

SAHAR SHARIFZADEH, Princeton University, Dept. of Electrical Engineering, PATRICK HÜANG, Physics and Life Sciences Directorate, Lawrence Livermore National Laboratory, EMILY A. CARTER, Princeton University, Dept. of Mechanical and Aerospace Engineering — At low temperatures, a variety of magnetic impurities adsorbed on metal surfaces form a Kondo state, where the conduction electrons are thought to screen out the spin on the impurity to yield a many-body spin singlet, based on analogy with bulk Kondo physics in which magnetic quenching is observed at low temperatures. In scanning tunneling spectroscopy (STS), this state manifests as a narrow resonance in the density of states at the Fermi level. However, qualitative differences in the Kondo resonance lineshape are seen between specific adatom-substrate systems, for reasons that are not understood. We present a many-body correlated wavefunction study of Co on transition metal surfaces. We apply an embedded configuration interaction (CI) approach, where a finite cluster containing the impurity is described by a many-body CI wavefunction, while the effects of the extended background are included via a periodic density functional theory-based embedding potential. We discuss the nature of the correlated wavefunction and impurity orbital structure on different surfaces, and discuss implications for the observed STS data.

12:03PM W11.00005 Kondo effect in single-molecule magnet transistors

GABRIEL GONZALEZ, MICHAEL LEIJENBERGER, NanoScience Technology Center, Univ Central Florida, EDUARDO MUCCIOLO, Department of Physics, Univ Central Florida — We present a careful and thorough microscopic derivation of the anisotropic Kondo Hamiltonian for single-molecule magnet (SMM) transistors. When the molecule is strongly coupled to metallic leads, we show that by applying a transverse magnetic field it is possible to topologically induce or quench the Kondo effect in the conductance of a SMM with either an integer or a half-integer spin $S=1/2$. This topological Kondo effect is due to the Berry-phase interference between multiple quantum tunneling paths of the spin. We calculate the renormalized Berry-phase oscillations of the two Kondo peaks as a function of a transverse magnetic field by means of the poor man’s scaling approach. We illustrate our findings with the SMM Ni4, which we propose as a possible candidate for the experimental observation of the conductance oscillations.

12:15PM W11.00006 Frequency-dependent Full Counting Statistics of Electron Transport in Double Quantum Dots

RAMON AGUADO, DAVID MARCOS, CSIC, CLIVE EMARY, TOBIAS BRANDES, Technische Universität Berlin — Full Counting Statistics is a powerful tool to study correlations in stochastic processes. It has been applied in the last years to characterize nanoscale transport. We present a technique that allows to calculate frequency dependent high-order correlators of the electronic current through an interacting nanostructure. We illustrate our technique by calculating the frequency-dependent shot noise (second order) and skewness (third order) of a double quantum dot. Our results demonstrate that the frequency- dependent skewness contains useful information about the interaction quantum dynamics of the nanostructure in bias voltage regimes where the second-order correlations are dominated by thermal fluctuations.

12:27PM W11.00007 Transport properties of a superconducting single-electron transistor coupled to a nanomechanical oscillator

VERENA KOERTING, T.L. SCHMIDT, C.B. DOIRON, C. BRUDER, Department of Physics, University of Basel, CH-4056 Basel, Switzerland, B. TRAUZETTEL, Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — Superconducting single-electron transistors (SSETs) are known to constitute a very sensitive probe for the position measurement of a nanomechanical resonator (NR) which can provide near quantum-limited accuracy. The laws of quantum mechanics, however, also require a backaction of the SSET on the resonator, which limits the sensitivity. Recent experiments have confirmed that the backaction gives rise to an effective thermal bath which has the potential to cool or drive the resonator. Our research attempts to gain a better understanding of this system by examining the action of the NR on the SSET. In particular, we investigate the effect on transport properties of the SSET. We focus on the double Josephson quasiparticle (DJQP) resonance where an especially strong backaction can be observed due to the tunneling of the two coherent Cooper pair tunneling events. We argue that a measurement of, for example the current, the charge noise and the shot noise (Fano factor) provides a direct way of gaining information on the state of the NR. In addition to an analytical discussion of the linear response regime we discuss results of higher order approximation schemes and a full numerical solution.

12:39PM W11.00008 Spin-dependent tunneling and the Kondo effect in quantum dots.* S. E. ULLOA, A. NGO, Ohio U, E. VERNEK, UFU-Brasil — Many-body effects have a significant role in electronic transport of nanoscale systems. Particular interesting systems are quantum dots coupled to electronic reservoirs via quantum point contacts. Due to strong spin-orbit interactions [1,2], quantum point contacts can exhibit spin dependent hybridization of the QD states, opening the possibility for generating spin-polarized transport. In this work we study electronic transport of a single level quantum dot coupled to polarizing quantum point contacts (QPCs) in both the Coulomb blockade and Kondo regimes. We study how QPC gate voltage dependence spin-polarized current is using scattering matrix methods and the equations-of-motion technique. We calculate the electronic Green’s function, conductance and spin polarization in different parameter regimes. Our results show that both Hubbard and Kondo regimes exhibit high spin-polarized conductance. We analyze how the spin-dependent hybridization of the QPC modifies the Kondo resonance, as well as the density of states of the system. These effects are controllable by lateral gate voltages applied on QPCs, as in recent experiments [2]. [1] A. Reynoso et al., Phys. Rev. B 75, 085321 (2007). [2] P. Debray et al., unpublished (2008). * Supported by NSF-DMR WNM.
Andreev transport through side-coupled double quantum dots, Yoichi TANAKA, Condensed Matter Theory Laboratory, RIKEN, Norio KAWAKAMI, Department of Physics, Kyoto University, Akira OGURI, Department of Material Science, Osaka City University — We study the transport through side-coupled double quantum dots, connected to normal and superconducting (SC) leads with a T-shape configuration, using the numerical renormalization group. We find that the Coulomb interaction in the side dot suppresses the destructive interference effect typical of the T-shape geometry, and enhances the conductance substantially in the Kondo regime. This behavior stands in stark contrast to a wide Kondo valley seen in the normal transport. Moreover, the SC proximity penetrating into the interfacial dot pushes the Kondo clouds, which screens the local moment in the side dot, towards the normal lead to make the singlet bond long. The conductance shows a peak of the unitary limit as the cloud expands. It is further elucidated that two separate Fano structures appear in the gate-voltage dependence of the Andreev transport, and the corresponding line shape is quite different from the Fano-Kondo plateau observed in the normal transport.

Zeeman vs resonance splitting effects in a double quantum dot system, N. SANDLER, Ohio U, E. VERNEK, UFU-Brasil, L.G.G.V. DIAS DA SILVA, ORNL-UT, R. INGERSENT, U Florida, S.E. ULLOA, Ohio U — Electron correlations in quantum dot (QD) systems have many intriguing consequences. At low temperatures, the coupling between confined and conduction electrons is known to realize the Kondo effect. This phenomenon exhibits new and interesting features when electrons in an interacting QD hybridize with a non-flat conduction band. For example, when the QD is side-connected to external leads via a second large (noninteracting) QD, the effective density of states coupling to the interacting QD can have a peak at or near the Fermi level. In this regime, interference between the many-body Kondo state in the interacting dot and the single-particle resonance on the other dot causes splitting of the Kondo resonance [1]. Here, we use the numerical renormalization group method to study this double-QD system in the presence of an external in-plane magnetic field. We explore the interplay between different energy scales and discuss the behavior of the Kondo resonance in the presence of competing interactions. The in-plane field suppresses the Kondo effect, although this requires a stronger field than for a single QD, and the conductance decreases with field in a non-universal fashion. [1] L. G. V. Dias da Silva et al., Phys. Rev. Lett. 97, 096603 (2006).

Shot noise in a Mn-doped quantum dot nanomagnet, L.D. CONTRERAS-PULIDO, ICM-CSIC, Spain, J. FERNANDEZ-ROSSIER, Universidad de Alicante, Spain, R. AGUADO, ICM-CSIC, Spain — A single-electron transistor (SET) based upon a II-IV semiconductor quantum dot doped with a single Mn ion behaves as a nanomagnet whose magnetic properties can be controlled electrically, and the effective exchange between the Mn and the carriers depends whether the SET is operated in the electron or the hole region. For holes, the Ising coupling for symmetric dots in absence of spin-flip Mn-hole exchange, results in Coulomb Blockade oscillations which depend on the spin state of the Mn atom [1]. We extended such analysis and studied finite-frequency shot noise through the SET [2]. Shot noise shows various regimes which, as a function of gate and bias voltages, reflect different magnetic configurations of the nanomagnet. We find super-Poissonian noise in a region of bias and gate voltages where the competing dynamics between slow and fast channels (corresponding to different orientations between the hole and the Mn ion) results in bunching. This behavior appears as a resonance around zero frequency, reflecting charge relaxation dynamics. We also discuss the role of transverse spin-flip terms. [1] J. Fernandez-Rossier and R. Aguado, Phys. Rev. Lett. 98, 106805 (2007) [2] D. Contreras-Pulido, J. Fernandez-Rossier and R. Aguado, in preparation

Kondo effects in triangular triple quantum dots, Akira OGURI, Takahide NUMATA, Yunori NISIKAWA, Osaka City University, A.C. HEWSON, Imperial College — We study the conductance through a triangular triple quantum dot, which is connected to two noninteracting leads, using the numerical renormalization group (NRG). It is found that the system shows a variety of Kondo effects depending on the filling of the triangle. The SU(4) Kondo effect occurs at half-filling, and a sharp conductance dip due to a phase lapse appears in the gate-voltage dependence. Furthermore, when four electrons occupy the three sites on average, a local S = 1 moment, which is caused by the Nagaoka mechanism, is induced along the triangle. The temperature dependence of the entropy and spin susceptibility of the triangle shows that this moment is screened by the conduction electrons via two separate stages at different temperatures. The two-terminal and four-terminal conductances show a clear difference at the gate voltages, where the SU(4) or the S = 1 Kondo effects occur [1]. We will also discuss effects of deformations of the triangular configuration, caused by the inhomogeneity in the inter-dot couplings and in the gate voltages.

Interference in triple quantum dot systems, George MARTINS, Oakland University, Edson VERNEK, Ohio University, Carlos BUSSER, Oakland University, Enrique ANDA, PUC - Rio - Brazil, Sergio ULLOA, Nancy SANDLER, Ohio University — Transport properties of an interacting triple quantum dot system coupled to three leads in a triangular geometry has been studied in the Kondo regime. Applying mean-field finite-U slave boson and embedded cluster approximations to the calculation of transport properties of this system unveils a set of very rich features associated to its particular symmetry. In the case where just two leads are present, interference effects between degenerate molecular levels are studied, as well as an S = 1 Kondo effect. The introduction of a third lead does not affect the coherence of propagating electrons, but rather results in an 'amplitude leakage' phenomenon, which alters the interference effects. There is a good overall agreement between the two techniques employed.

Bloch oscillations in lateral periodic nanostructure arrays, W. PAN, S.K. LYO, J.L. RENO, J.A. SIMMONS, Sandia National Labs, D. LI, S.R.J. BRUECK, CHTM, University of New Mexico — In a periodic structure of electron potential, under an external electric field E, if an electron can reach the boundary of the Brillouin zone (BZ) without being scattered, it undergoes Bragg reflection, passing back into the BZ on the opposite side. This results in a high frequency oscillation of electrons, i.e., Bloch oscillation (BO). Recently, BO has gained a renewed interest, as a Blochoscillator can be utilized as a frequency-tunable THz source. Work on BO has mainly been carried out in quantum well superlattices. On the other hand, a surface superlattices patterned into a two dimensional electron system has long been proposed as an alternative structure to generate BO. Here, we present our experimental results on the nonadiabatic differential conductance and Bloch oscillation induced edge magnetoplasma resonance in a series of lateral superlattices. Results from the so-called reversed Bloch oscillations measurements and bolometric measurements will also be presented and discussed. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin company, for the US Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. The facilities of the NSF-sponsored NNIN node at UNM were used for the fabrication.

Thursday, March 19, 2009 11:15AM - 2:15PM – Session W12 DMP DCMP: Steps, Islands and Nanostructures
11:15AM W12.00001 Relaxation of Terrace-width Distributions: Novel Analysis and Features

T.L. EINSTEIN, Univ. of Maryland, College Park (UM), AMJI BH. HAMOUnda, UM & Univ. Monastir, Tunisia, A. PIMPINELLI, U.M & U.B.P.Clermont-2 & Science Attaque, French Consulate, Houston — We describe a Fokker-Planck scheme to describe the relaxation of the terrace-width distribution (TWD) on a vicinal surface toward the generalized Wigner form describing equilibrium. We performed KMC calculations on the standard minimal SOS model to show that the time constant gives physical information, in particular the energy barrier of the rate-determining process. For close-packed steps, this involves kink-antikink generation, breaking 3 rather than the expected 2 lateral bonds (the latter associated with equilibrium fluctuations). We discuss strengths and limitations of this FP procedure, higher moments of the distribution beyond the variance, and generalizations to other step orientations.

1Work at UM supported by the MRSEC, NSF Grant DMR 05-20471

11:27AM W12.00002 Nanowires of Terrace-width Distributions During Growth on Vicinals

AMJI BH. HAMOUnda, Univ. of Maryland, College Park (UM) & Univ. Monastir, Tunisia, A. PIMPINELLI, UM & U.B.P.Clermont-2 & Science Attaque, French Consulate, Houston, T.L. EINSTEIN, UM — Using kinetic Monte Carlo simulations for a generic minimal SOS model of vicinal surfaces, we compute the terrace-width distributions (TWDs) as a function of incident flux during homoepitaxial growth. We show that the distribution narrows markedly as though there were a flux-dependent repulsion between steps, until the step picture fails at high flux. Using a Fokker-Planck approach, we analyze the evolution and saturation of this narrowing. We compare with a 1D model and with simulations for narrowing due to an Ehrlich-Schwoebel barrier.

1Work at UM supported by the MRSEC, NSF Grant DMR 05-20471.
4H.-J. Gossman et al., J. Appl. Phys. 67 (1990) 745

11:39AM W12.00003 Stability and mobility of vacancy nanoclusters on Cu(111) surface: An ab initio study

ALIREZA AKBARZADEH, ZHENGZHENG CHEN, NICHOLAS KIOUSSIS, California State University Northridge, Department of Physics & Astronomy, 18111 Northridge, CA 91330-8268 — We used ab initio calculations to study stability and mobility of vacancy nanoclusters on Cu(111) surface. We found that the formation energies for single vacancies in the vicinity of surface are ≈0.3 eV lower than that in bulk. Interestingly, calculations yield strongly bonded 1^2NN vacancy on the surface than in bulk. In addition a vacancy binds very strong on the surface, indicating that formation of loop-like vacancy nanoclusters are most energetically favored on the surface. These findings imply the ease of nucleation of vacancy nanoclusters on the surface. We also examined migration of mono-, di- and trivacancy on the surface. A zagzag motion for divacancy diffusion on the surface is predicted with the migration barrier higher on the surface than in the bulk due to larger binding energy and elastic contribution.

1This research is supported by the National Science Foundations under grant NSF-NIRT CMS-0506841.

11:51AM W12.00004 Two-dimensional island ripening on the basal plane of ice

SHU NIE, NORM BARTEL, KONRAD THURMER, Sandia National Labs, SANDIA NATIONAL LABORATORIES TEAM — Despite the importance of ice surfaces to many natural phenomena there have been no accurate measurements of surface self-diffusion coefficients of ice. To provide this needed basic information, we applied the newly discovered capability of STM to image thick ice films on Pt [1], and tracked the evolution of 2-dimensional ice islands grown on the basal plane of ice. Uniform 5 nm thick ice films grown at 145 K were used as a template to study surface self-diffusion. By depositing a fraction of a monolayer of water onto these films at 115 K, we created arrays of two-dimensional islands with diameters of 5-10 nm. Remarkably, when annealed to temperatures between 115 and 135 K, these island arrays coarsened. By fitting the average island area to the $t^{2/3}$ growth law expected for diffusion-controlled ripening we extract an activation energy for surface self-diffusion of 0.4 ±0.1 eV, which is on the order of the energy of a hydrogen bond and much less than the value measured for bulk diffusion (0.7 eV) [2]. This work is supported by U. S. DOE, OBES, Division of Materials Sciences under contract DE-AC04-94AL8500. [1] K. Thürmer and N. C. Bartel, Phys. Rev. B 77, 195425 (2008). [2] D. E. Brown and S. M. George, J. Phys. Chem. 100, 15460 (1996).

12:03PM W12.00005 Ferromagnetic-Semiconductor Interfacial Order Suppression: Self-Assembled Fe$_x$Ga Island Structures on GaAs(001)

PHILIP RYAN, JONG WOO KIM, Ames Laboratory, JUSTIN SHAW, National Institute of Standards and Technology, CHARLES FALCO, University of Arizona, LAHSEN ASSOUFID, RICHARD ROSENBERG, DAVID KEAVNEY, Argonne National Laboratory, AMES LABORATORY TEAM, NIST COLLABORATION, UNIVERSITY OF ARIZONA COLLABORATION, ARGONNE NATIONAL LABORATORY COLLABORATION — The practical development of spintronics requires a new class of multifunctional microelectronic components, involving electronic device mechanisms dependent upon ferromagnetic materials. The Fe-GaAs(001) system has been extensively studied as the prototypical spin injection junction for spintronic device mechanisms. Increasing spin injection efficiency has been calculated to be dependent upon the structural order of an abrupt interfacial junction between a ferromagnet and semiconductor. Room temperature low coverage Fe deposition on GaAs(001) reveals the formation of fully strained, epitaxial Fe$_x$Ga domains. An iron interfacial layer adheres fully coherent to the buried substrate surface. The adlayer is mediated through the back-bonding of the Fe to substrate terminating As. This structural environment is tied to the suppression of interfacial order.

12:15PM W12.00006 Snow flake shaped gold nanostructures templated on graphene: an avenue to fabricate novel nano electronic devices

KABEER JASUJA, VIKAS BERRY, Kansas State University — Non spherical gold nanoparticles such as rods, multipods, polygons, cubes, stars and branched nanostructures have generated significant research attention in the past few years. Such anisotropic nano structures have been shown to exhibit size and shape dependent properties which are either significantly different or highly pronounced from their spherical counterparts. The unique properties of anisotropic nanostructures (such as localized surface plasmon resonance and surface enhanced fluorescence) make these ideal candidates for a broad range of emerging applications in photonics, opto-electronics, biomedical labeling, sensing and imaging. One of the foremost challenges in utilizing such properties is integrating the anisotropic gold nanostructures into devices which can justifiably tap these properties. Here we demonstrate a simple colloidal synthetic route that results in the formation of snow-flake shaped nanostructures of gold (Au SFs) templated on the nano-sheets of Graphene-oxide(GO). Graphene nanosheets have generated renewed interest in recent years due to their unique 2-dimensional nature and associated electronic, physical and chemical properties. An assembly of Au SFs supported on GO sheets will not only give way to the next generation electronic and optoelectronic nanodevices but will also find wide ranging applications in a number of industrially relevant reactions such as catalysis, fuel cell technology and pollution control.
12:27PM W12.00007 Large-area nanocrystal superlattice films by surface-tension mediated self-assembly. ANGANG DONG, CHRISTOPHER MURRAY, University of Pennsylvania — We report a facile and general approach based on the dynamic self-assembly of nanocrystals on the liquid/liquid interface to fabricate hierarchically ordered nanocrystal superlattices with thicknesses up to several centimeters. In addition to the close-packed ordering of nanocrystals at nanometer scale, the film exhibits exceptionally ordered stripe patterns at micrometer scale. The stripes are formed by the controlled, repetitive stick-slip motion of the liquid-liquid contact line. Both the film thickness and the stripe periodicity are tunable by changing the nanocrystal concentration. The final nanocrystal film, supported on the liquid surface, can be readily transferred to arbitrary substrates for device fabrication. The methodology reported here not only provides a simple and highly reproducible approach for production of large-area nanocrystal superlattice films, but also opens up a new avenue for lithography-free patterning of nanocrystal arrays for applications in optical, electronic, and magnetic devices.

12:39PM W12.00008 Mechanism of Asymmetric Growth of Wurtzite Nanostructures: A Case Study of CdSe Through Ab Initio Computations. GHANSHYAM PILANIA, RAMAMURTHY RAMPRASAD, University of Connecticut — An interesting and potentially useful phenomenon observed in wurtzite semiconductor nanocrystals is asymmetric anisotropic growth. This property has been exploited in the preferential creation of nanorods, nanoribbons and nanosaws over spherical nanocrystals. However, the details of the mechanism underlying this phenomenon of asymmetric anisotropic growth remain poorly understood. Here, we use CdSe as a prototypical wurtzite system, and oxygen as an agent that encourages asymmetric anisotropic growth. This study focus on the impact of the ordering of the surface energies of several polar and nonpolar surface facets as a function of (i) the chemical potential of Cd (i.e., precursor concentration), (ii) the presence of oxygen adsorbates, (iii) the binding modes of oxygen at the surface, and (iv) the density of oxygen adsorbates on the surfaces, using density functional theory (DFT). Our results show that by controlling the ordering of the surface energies (e.g., through proper choices of precursor concentration, temperature, and surfactants), novel growth modes such as asymmetric growth can be made possible.

12:51PM W12.00009 Ab Initio Study of the Effects of Surface Chemistry and Size on Xray Absorption Spectra of CdSe Nanoparticles. HEATHER WHITLEY, Lawrence Livermore National Laboratory, Livermore, CA 94551, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, TADASHI OGITSU, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, CA 94551 — The specificity of their opto-electronic properties with respect to size, shape, and surface chemistry, as well as cost-effective sol-gel methods of synthesis, make CdSe nanoparticles a material of choice for use in novel opto-electronic devices, such as photovoltaics and field effect transistors. Developing methods by which these nanomaterials can be systematically engineered to meet specific device goals is largely dependent on understanding how surface passivation and reconstruction affect the properties of a given nanomaterial. Xray absorption spectroscopy (XAS) is an ideal method for structural analysis, but its application to studying nanomaterial surfaces is nontrivial due to the convolution of the absorption of surface atoms with those within the nanomaterial. We utilize ab initio methods to investigate the dependence of the Cd L-edge x-ray absorption cross-section on the size and passivation of Cd atoms both at the surface and within the core of CdSe nanomaterials. We aim to enable routine surface characterization of CdSe nanomaterials via XAS. Prepared by LLNL under Contract DE-AC52 07NA27344.

1:03PM W12.00010 Microwave induced in-situ deposition of Gold and Silver nanoparticles on chemically modified sheets of graphene: Avenue to build Graphene-metal interface. KABEER JASUSA, VIKAS BERRY, Kansas State University — In recent years there has been a great interest in the architecture of 2-D sheets of graphene which have been shown to display remarkable electronic, physical and chemical properties. An extremely high conductivity of graphene sheets along with the ease these can be prepared, has already made graphene as the material of choice for applications in several electronic, optoelectronic and biodevices. There is a great deal of interest in interfacing graphene sheets with other low dimensional nanostructures for building novel hybrids. Coupling such low dimensional materials at nano scale yield novel composites with interesting properties. In this study we synthesized nanoparticles of gold and silver on the sheets of graphene-oxide using a one step microwave heating method. Our results indicate that the sheets of chemically modified graphene act as excellent templates for in-situ formation of gold and silver nanoparticles. The advantage of this present synthetic route lies in not using the conventional low molecular weight stabilizing agents which can otherwise react with the graphene sheets leading to impurities. This simple processing approach opens up a new way to synthesize hybrid sheets of graphene decorated with gold and silver nanoparticles which can be used in developing novel catalysts and composites.

1:15PM W12.00011 Efficient sticking of surface-passivated Si nanospheres via phase-transition plasticity. TRAIAN DUMITRICA, MAYUR SURI, University of Minnesota — Large-scale atomistic simulations considering a 5 nm in radius H-passivated Si nanosphere that impacts with relatively low energies onto a H-passivated Si substrate reveal a transition between two fundamental collision modes. At impacting speeds of less than ~ 1000 m/s, particle-reflection dominates. At increased speeds the partial onset in the nanosphere of a β-tin phase on the approach followed by α-Si phase on the recoil is an efficient dissipative route that promotes particle-capture. In spite of significant deformation, the integrity of the deposited nanosphere is retained. Our result explains the efficient fabrication of nanoparticulate films by hypersonic impact, where the nanoparticle impact velocities equal 1000–2000 m/s.


1:27PM W12.00012 Electronic Nano-Structures as Ionic Barriers: A New Corrosion Prevention Concept. SREEYA SREEVATSA, Department of Applied Physics and the Electronic Imaging Center, HAIM GREBEL, Department of Electrical and Computer Engineering and the Electronic Imaging Center — Corrosion is a longstanding problem which costs the economy billions of dollars annually. The simplest way to prevent corrosion is to use paint thereby blocking diffusion of corrosive component towards the metallic surface. Here we consider a new concept - the electronic barrier – for corrosion prevention. The barrier is an electronic p-n junction made by topping one film of functionalized carbon nanotubes on another. The barrier is constructed such that the positive ions in the electrolyte are prohibited from reaching the metallic surface through electronic screening.

1:39PM W12.00013 Ion-beam-assisted nano-texturing of halite-structure thin films. VLADIMIR MATIAS, Los Alamos National Laboratory — We study biaxial crystalline texturing at early film growth in a variety of compounds during ion-beam-assisted deposition (IBAD). We have found that many different halite-structure compounds share the ion-beam texturing ability at nucleation and early film growth. This includes numerous oxides and nitrides. Fluorite-structure compounds also exhibit the possibility of fast IBAD texturing. For these materials IBAD texturing can be achieved within the first few nanometers of deposited material. We examine the detailed texture evolution for MgO. To perform these experiments we developed a unique experimental methodology based on linear combinatorial research. Three different texture development regions can be identified in MgO texture evolution. The first stage where biaxial texture first appears is during grain nucleation. With additional IBAD texture continues to improve by grain alignment up to a certain point. Further improvement in crystalline alignment can be achieved by a third stage of epitaxial overgrowth. We find that the IBAD texture development is very sensitive to the nucleation surface conditions, both chemical species and surface morphology. An in-plane texture of less than 0.5° and an out-of-plane texture of less than 1° are attainable in an artificially textured MgO layer on an amorphous substrate. This work is supported by the DOE Office of Electricity Delivery & Energy Reliability.
11:15AM W13.00001 Electronic structure of electron doped Ba$_2$Fe$_2$As$_2$ superconductors revealed by Angle Resolved Photoemission. P. VILMERCATI, I. VOBRONIK, M. UNNIKRISHNAN, A. FEDOROV, A. GOLDONI, G. PANACCIONE, A. SAFAFEFAT, R. JIN, M.A. MCGUIRE, B.C. SALES, D.J. SINGH, D. MANDRUS, N. MANNELLA — The electronic structure in the normal state of Co-doped Ba$_2$Fe$_2$As$_2$ superconductors has been measured by Angle Resolved photoemission (ARPES). Co doping on the Fe site results in electron doping [A. S. Sefat et al., Phys. Rev. Lett. 101, 117004 (2008)]. The data qualitatively reveal that Co-doping results in raising the chemical potential, as expected with electron doping. The Fermi surface topology and the possible relevance to the mechanism of spin fluctuation will also be discussed.

11:27AM W13.00002 ARPES Study of the Electronic Structure of the Fe Pnictides. MING YI, DONGHUI LU, RUIHUA HE. Stanford University, SUNG-KWAN MO. Advanced Light Source, LBNL, JAMES ANALYTIS, JUIN-HAW CHU, ANN ERICKSON, Stanford University, DAVID SINGH, Material Science and Technology Division, Oak Ridge National Lab, ZAHID HUSSAIN, Advanced Light Source, LBNL, TED GEBALLE, IAN FISHER, Stanford University, XINGJIANG ZHOU, G.F. CHEN, JIANLIN LUO, NANLIN WANG, Institute of Physics, Chinese Academy of Sciences — Recently superconductivity has been discovered in many iron pnictides when they are properly doped with charge carriers. Thus it is expected with electron doping. The Fermi surface topology and the possible relevance to the mechanism of spin fluctuation will also be discussed.

11:39AM W13.00003 Study of band structure and Fermi Surface of SrFe$_2$As$_2$ and BaFe$_2$As$_2$ by angle-resolved photoemission spectroscopy. MADHAB NEUPANE, Y.-M. XIU, Z. WANG, Boston College, P. RICHARD, S. SOUMA, WPI Research Center, Tohoku University, K. NAKAYAMA, Tohoku University, T. SUGAWARA, Tohoku University., T. ARAKANE, Y. SEKIBA, A. TAKAYAMA, T. SATO, T. TAKAHASHI, Tohoku University, X. DAI, Z. FANG, G.F. CHEN, J.L. LUO, J. BOWEN, N.L. WANG, H. DING, Institute of Physics, Chinese Academy of Sciences — Recently superconductivity has been discovered in many iron pnictides when they are properly doped with charge carriers. Thus it is important to understand the undoped parent compounds that also have a puzzling collinear antiferromagnetic ground state. We have performed a systematic angle-resolved photoemission study on some of the parent compounds, mostly on SrFe$_2$As$_2$ and BaFe$_2$As$_2$, to investigate their electronic structure and Fermi surface. We will report our experimental results and the comparisons to first-principle band calculations.

11:51AM W13.00004 Fermi surface and superconducting gap of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ studied by high-resolution ARPES. K. NAKAYAMA, T. SATO, Y. SEKIBA, Tohoku University, P. RICHARD, S. SOUMA, WPI, Tohoku University, M. NEUPANE, Y.-M. XIU, Z. WANG, Boston College, X. DAI, Z. FANG, G. F. CHEN, J. L. LUO, N. L. WANG, H. DING, Chinese Academy of Sciences, T. TAKAHASHI, WPI, Tohoku University — The electronic states near the Fermi level are the key ingredient to understand the superconducting mechanism of iron-based superconductor. Although electrons in the iron orbitals have been found to play a key role to the occurrence of the superconductivity, the microscopic origin of high-$T_c$ superconductivity is still unclear. To address this important issue, we report our recent high-resolution ARPES results on hole-doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$, and demonstrate the Fermi-surface-sheet and momentum dependence of the superconducting gap as well as the doping evolution of the Fermi surface and band structure.

12:03PM W13.00005 ARPES study of doping dependence of the superconducting gap in Ba$_{1-x}$K$_x$Fe$_2$As$_2$. Y.-M. XIU, M. NEUPANE, Department of Physics, Boston College, P. RICHARD, WPI Research Center, Advanced Institute for Material Research, Tohoku University, K. NAKAYAMA, Y. SEKIBA, Department of Physics, Tohoku University, T. QIAN, S. SOUMA, WPI Research Center, Advanced Institute for Material Research, Tohoku University, T. SATO, T. TAKAHASHI, Department of Physics, Tohoku University, H.-H. WEN, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Z. WANG, Department of Physics, Boston College, H. DING, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences — High transition temperature superconductivity has been discovered recently in many doped iron pnictides which join the cuprates in the family of high-$T_c$ superconductors. It is very important to understand the nature of the superconducting gap and its doping dependence, as in the case of the cuprates, in order to understand this new class of superconductors. A systematic angle-resolved photoemission spectroscopy (ARPES) study has been performed on the iron pnictide Ba$_{1-x}$K$_x$Fe$_2$As$_2$ at different K concentrations, to determine its doping dependence of the superconducting gap. We will report our ARPES results and their implications.
12:15PM W13.00006 Momentum dependence of superconducting gap, strong-coupling dispersion kink, and tightly bound Cooper pairs in the high-Tc (Sr,Ba)1-x(K,Na)xFe2As2 superconductors, LEWIS WRAY, DONG QIAN, DAVID HSIEH, YUQI XIA, ALI YAZDANI, N. PHUAN ONG, Princeton University, NANLIN WANG, Beijing National Laboratory for Condensed Matter Physics, M. ZAHID HASAN, Princeton University — We present a systematic angle-resolved photoemission spectroscopic study of the high-Tc superconductor class (Sr,Ba)1-x(K,Na)xFe2As2. By utilizing a photon-energy-modulation contrast and scattering geometry we report the Fermi surface and the momentum dependence of the superconducting gap, \( \Delta(T) \). A prominent quasiparticle dispersion kink reflecting strong scattering processes is observed in a binding-energy range of 25-55 meV in the superconducting state, and the coherence length or the extent of the Cooper pair wave function is found to be about 20 \( \AA \), which is uncharacteristic of a superconducting phase realized by the BCS-phonon-retardation mechanism. The observed 40-2.15 meV kink likely reflects contributions from the frustrated spin excitations in a J1-J2 magnetic background and scattering from the soft phonons. Results taken collectively provide direct clues to the nature of the pairing potential including an internal phase-shift factor in the superconducting order parameter which leads to a Brillouin zone node in a strong-coupling setting.

12:27PM W13.00007 Momentum dependence of the superconducting gap in NdFeAsO\(_{1−x}\)F\(_x\) single crystals measured by angle resolved photoemission spectroscopy, TAKESHI KONDO, A.F. SANTANDER-Syro, O. COPIE, CHANG LIU, M.E. TILLMAN, J. SCHMALIAN, S.L. Bud'ko, P.C. CANFIELD, A.D. Kaminiski, Nanlab and Dept. of Physics and Astronomy, Iowa State University — We use angle resolved photoemission spectroscopy (ARPES) to study the momentum dependence of the superconducting gap in NdFeAsO\(_{1−x}\)F\(_x\) single crystals. We find that the T' hole pocket is fully gapped below the superconducting transition temperature. The value of the superconducting gap is 15 ± 3 meV and its anisotropy around the hole pocket is smaller than 20% of this value. This is consistent with an isotropic or anisotropic s-wave symmetry of the order parameter or exotic d-wave symmetry with nodes located off the Fermi surface sheets. This is a significant departure from the situation in the cuprates, pointing to possibility that the superconductivity in the iron arsenic based system arises from a different mechanism.

12:39PM W13.00008 3D band structure determination of BaFe2As2, CaFe2As2 and SrFe2As2, QIANG WANG, ZHE SUN, Department of Physics, University of Colorado Boulder, FILIP RONNING, ERIC BAUER, Los Alamos National Laboratory, SUCHITRA SEBASTIAN, Cavendish Lab, Cambridge, UK, DANIEL DESSAU, Department of Physics and JILA, University of Colorado Boulder — The band structure of the parent compounds of iron-arsenic superconductors BaFe2As2, CaFe2As2 and SrFe2As2 are investigated by angle-resolved photoemission spectroscopy. The dispersion of predominant Fe 3d bands has been successfully resolved and compared with theoretical calculations. Although the overall band structure is in line with nonmagnetic DFT computations, the Fe 3d band dispersions strongly deviate from calculations, and the Fermi surface topology differs from theoretical results. These results suggest that some significant correlations have not been correctly involved in the current understanding of these new materials. The kz dependence of the Fermi surface structure has also been studied for these quasi-2D materials.

12:51PM W13.00009 Band Structure and Fermi Surface of Extremely Overdoped Iron-Based Superconductors, TAKAFUMI SATO, K. NAKAYAMA, Y. SEKIBA, Dep. Physics, Tohoku University, P. RICHARD, S. SOUMA, WPI, Tohoku University, Y.-M. XU, Boston College, G. F. CHEN, J. L. LUO, N. L. WANG, H. DING, Chinese Academy of Sciences, T. TAKAHASHI, WPI and Dep. Physics, Tohoku University — The discovery of superconductivity at 26 K in LaFeAsO\(_{1−x}\)F\(_x\) has triggered intensive researches on the high-temperature (\( T_c \)) superconductivity of iron pnictides and opened a new avenue for high-\( T_c \) material research beside cuprates. To elucidate the mechanism of high-\( T_c \) superconductivity in terms of the electronic structure, previous angle resolved photoemission spectroscopy (ARPES) studies have been performed on both hole and electron-doped compounds in the optimally- or non(under)-doped region. On the other hand, little is known about the electronic states in the overdoped region. We report ARPES measurements on heavily overdoped pnictides. Our results indicate that the electronic states around the M point play an important role in the high-\( T_c \) superconductivity of these materials and suggests that the interband scattering via the antiferromagnetic wave vector essentially controls the \( T_c \) value in the overdoped region.

1:03PM W13.00010 Electronic structure of electron-doped BaFe\(_2\)−\(_x\)Co\(_x\)As Superconductor class studied by ARPES, DONG QIAN, princeton university, N.L. WANG, Institute of Physics, Chinese Academy of Sciences, M.Z. HASAN, princeton university — State-of-art high resolution angle-resolved photoemission spectroscopic studies have been carried out on the electron doped BaFe\(_2\)−\(_x\)Co\(_x\)As Superconductor (Tc=26K). Electronic band structure, Fermi surface topology and superconducting gap evolution would be reported in this presentation. Nature of the spin sensitivity wave (SDW) state would be discussed from a band nesting point of view.

1:15PM W13.00011 Observation of an orbital selective electron-mode coupling in Fe-based high-Tc superconductors, PIERRE RICHARD, WPI, Tohoku University, T. SATO, K. NAKAYAMA, Dep. Physics, Tohoku University, S. SOUMA, WPI, Tohoku University, Y.-M. XU, Boston College, G.F. CHEN, J.L. LUO, N.L. WANG, H. DING, Chinese Academy of Sciences, T. TAKAHASHI, WPI and Dep. Physics, Tohoku University — The recent discovery of Fe-based superconductors with critical temperatures up to 56 K raises the prospect of unconventional superconducting pairing mechanism. While the electronic pairing in conventional superconductors is mediated by phonons, its nature in the Fe-based high-Tc superconductors is unknown. A direct signature of an electron-mode coupling is an anomaly in the electronic energy dispersion (kink). For example, previous angle-resolved photoelectron spectroscopy (ARPES) studies revealed a kink in cuprates, which is believed to be linked to the pairing. We report an ARPES observation of a kink around 25 meV in the dispersion of superconducting Ba\(_{0.6}\)K\(_{0.4}\)Fe\(_2\)As\(_2\) that nearly vanishes above \( T_c \). The energy scale of the related mode (13±2 meV) and its strong dependence on orbital and temperature indicates that it is unlikely related to phonons. Moreover, the momentum locations of the kink can be connected by the antiferromagnetic wavevector. Our results point towards an electronic origin of the mode and the superconducting pairing in the Fe-based superconductors, and strongly support the anti-phase s-wave pairing symmetry.

1:27PM W13.00012 Electronic properties of CaFe\(_2\)As\(_2\), CHIANG LIU, TAKESHI KONDO, ARI PALCZEWSKI, GERMAN SAMOYUK, YONGBIN LEE, NI NI, SERGEY BUD'KO, PAUL CANFIELD, ADAM KAMINSKI, Ames Laboratory and Iowa State University, AARON BOSTWICK, ELI ROTENBERG, Advanced Light Source, Berkeley National Laboratory — CaFe\(_2\)As\(_2\) is a parent compound of a new family of FeAs based high-Tc superconductors. It undergoes a first-order structural transition from low-\( T \) orthorhombic to high-\( T \) tetragonal phase [Ni et al., Phys. Rev. B 78, 014523]. Moderate pressure lowers the transition temperature, and turns on the superconductivity [Toriguchii et al., Phys. Rev. Lett. 101, 057006]. Study on its electronic properties is of crucial importance for understanding the pairing mechanism of the FeAs based superconductors. Here we present angle-resolved photoemission spectroscopy (ARPES) results on both the orthorhombic and the tetragonal phase of CaFe\(_2\)As\(_2\). In the orthorhombic phase, we find strong \( k_z \) dispersion on the Fermi surfaces, showing a three dimensional electronic structure. We also find dramatic difference of the Fermi surface structure between the orthorhombic and the tetragonal phase.
1.39PM W13.00013 Fermi surface of the parent compound of iron-based superconductor, T. SHIMOJIMA, ISSP U. Tokyo, Y. ISHIDA, RIKEN SPRing-8, N. KATAYAMA, K. OHGUSHI, K. ISHIZAKA, T. KISS, M. OKAWA, ISSP U. Tokyo, T. TOGASHI, RIKEN SPRing-8, X.-Y. WANG, C.-T. CHEN, CAS, S. WATANABE, ISSP U. Tokyo, T. OGUCHI, U. Hiroshima, S. SHIN, ISSP U. Tokyo — Fermi surface of the parent compound of iron-based superconductor BaFe2As2 is studied by angle-resolved photoemission spectroscopy using VUV-laser. This compound shows structural and magnetic phase transition around TN = 140 K [1]. We found the transformation of Fermi surface across TN. We will discuss its origin comparing with the first principle band calculation.


1.51PM W13.00014 APRES study of in-plane element substituted iron-based superconductors Ba(Fe1-xCo$_x$)$_2$As$_2$ and Ba(Fe1-xNi$_x$)$_2$As$_2$, JONATHAN BOWEN, Institute of Physics, Chinese Academy of Sciences, KENSEI TERASHIMA, PIERRE RICHARD, TAKAFUMI SATO, TAKASHI TAKAHASHI, Tohoku University, ZHUAN XU, Zhejiang University, HONG DING, Institute of Physics, Chinese Academy of Sciences — Much excitement has surrounded the recent discovery of the doped pnicnides which exhibit high temperature superconductivity. These new materials are generally grouped into either 1111 or 122 compounds by the stoichiometric formula of the parent compounds. Understanding how doping with different valence affects their superconducting properties is a vital element of working toward a complete picture of these interesting new compounds. To that end, we have conducted a high-resolution APRES study of two 122 compounds: Ba(Fe1-xCo$_x$)$_2$As$_2$ and Ba(Fe1-xNi$_x$)$_2$As$_2$ and will report our results.


11:15AM W14.00001 Clustering in a Dense, Freely-Falling Granular Stream, JOHN R. ROYER, SCOTT R. WAITUKAITIS, James Franck Institute, University of Chicago, DANIEL J. EVANS, HEINRICH M. JAEGER, James Franck Institute, University of Chicago — We investigate the breakup of a freely-falling granular stream into discrete, compact clusters of grains. This breakup, occurring for grain diameters less than about 200 microns falling out of a hopper opening, is reminiscent of the breakup of a liquid stream, though granular materials are generally thought of as lacking a surface tension. Our experiments employ high-speed video imaging in the co-moving frame, which allows us to track the onset of clustering and the subsequent cluster evolution in detail. Varying the material, size, roughness, and wetting properties of the grains as well as the surrounding gas pressure and the hopper opening diameter, we investigate the role of capillary, electrostatic and van der Waals forces in the clustering process. We find that the clustering provides a window to observe very weak cohesive forces between the grains which are masked in other experiments.

1Supported by NSF through DMR-MRSEC and by the W. M. Keck Foundation.

11:27AM W14.00002 Vector Force Measurements of a Dense Granular Flow, KEVIN FACTO, University of Massachusetts-Amherst, TOM SCHICKER, NARAYANAN MENON, University of Massachusetts-Amherst — We have made force measurements at the wall of a dense granular flow. The data was acquired with planar elements at rate of 800 Hz in all three spatial directions. The fluctuations in the forces were examined for a wide range of flow speeds. Correlations in the forces decay by the time the flow moves one ball diameter. The force along the flow direction is highly correlated with the force normal to the wall. For a given value of normal force, the force along the flow has a gaussian distribution about the tangential force that would be predicted from a constant friction angle.

1Supported by NSF DMR-0606216 and NSF CBET-0651397

11:39AM W14.00003 Space-Time Structure of Granular Flows in a Rough Vertical Channel, DONALD CANDELA, KEVIN FACTO, University of Massachusetts Amherst — We report measurements using PFG-NMR of the space and time structure of steady granular flows through a long vertical channel of circular cross section with roughened walls. The granular sample consisted of seeds approximately 400 μm in diameter, flowing through a 9.8 mm ID tube to which was adhered a monolayer of glass beads similar in diameter to the grains. Data was acquired from a region approximately 50 channel diameters higher than the aperture at the channel bottom used to control the flow rate. The mean velocity of the grains as well as the RMS fluctuations in the grain motion were measured as functions of the radial coordinate and for time intervals in the range 5-200 ms, for several different granular flow speeds. For some flow regimes the displacement distributions are distinctly non-Gaussian, at odds with a “molecular fluid” model of the granular medium. The time dependence of the fluctuation distribution provides clues to the mechanism by which the gravitational body force is transmitted to the channel walls.

1Supported by NSF Grant CBET-0651397

11:51AM W14.00004 Vibrhology of Granular Matter, JOSHUA DIJKSMAN, GEERT WORTEL, MARTIN VAN HECKE, Leiden University — We show how weak agitations substantially modify the rheology of granular materials. We experimentally probe dry granular flows in a weakly vibrated split-bottom shear cell – the weak vibrations act as the agitation source. By tuning the applied stress and vibration strength, and monitoring the resulting strain, we uncover a rich phase diagram in which non-trivial transitions separate a jammed phase, a creep flow case, and a steady flow case.

12:03PM W14.00005 Shear zones at the walls of a 2D gravity-driven flow of grains, KELSEY HATTAM, NALINI EASWAR, Smith College, Northampton, MA, NARAYANAN MENON, University of Massachusetts, Amherst, MA — We study the flow of spherical grains under gravity in a vertical, straight-walled 2-dimensional hopper, where the flow velocity is controlled by a taper at the outlet. We perform these studies both for monodisperse steel spheres as well as for a bidisperse system of equal numbers of spheres with a ratio of diameters of 1.25. The monodisperse system shows crystalline order even in flow, whereas there is no obvious structural order in the bidisperse system. The velocity profile across the flow is profoundly different in the two systems: the wall shear zone in the monodisperse system extends only a few particle diameters, and there are only small velocity gradients in the bulk of the flow. In contrast to this nearly-plug-like flow, there are significantly broader shear zones in the disordered flow. We report these profiles as a function of the width of the hopper in order to study the scaling of the shear zone with the system size, and with the flow rate.

1Supported by NSF DMR 0606216 and NSF MRSEC DMR 0213695
12:15PM W14.00006 A Void Diffusion Model of Granular Flow  JAYANTA RUDRA, PAUL VIETH, Oklahoma School of Science and Mathematics — In an earlier paper1 we derived a nonlinear diffusion equation to describe the dynamics in granular flow based on a Diffusion Void Model (DVM). The equation was successfully used to describe the flow of a homogeneous granular material through the hole of a container under gravity. It also properly described similar flow in the presence of a flat horizontal barrier placed above the hole. Recently, however, we have found that the above nonlinear equation does not lead to correct static equilibrium. For example, the stability of the free surface of a granular aggregate cannot be described by the equation. The equation also fails to describe, say, how an unstable vertical column of a granular material will change to a stable A-shaped pile at the angle of repose. In this paper work we derive an equation using an appropriate current density of voids that can explain all the observed dynamical characteristics of a simple granular state. 1 Jayanta K. Rudra and D. C. Hong, Phys. Rev. E47, R1459 (1993).

12:27PM W14.00007 The Role of Extensional Viscosity in Sedimentation of Dense Suspensions THEODORE BRZINSKI, DOUGLAS DURIAN, University of Pennsylvania — When two particles in a viscous fluid approach contact the motion of the interstitial fluid is dominated by extensional flows. We are interested in how the details of these flows influence the sedimentation of sense suspensions. To highlight the effects of extensional flows on particle motion we compare systems in which the fluids have the same shear viscosities, but drastically different extensional viscosities. We enhance the extensional viscosity by adding a flexible, high molecular weight polymer. In the case of a system without polymer there is a dense, static packing which grows from the bottom of the container, a region which remains at the initial grain density and settles at a constant velocity, and a clear supernatant at the top. In the polymeric fluid particles settle more slowly, and rather than sedimenting directly from the initial density to a static packing there is a long consolidation process during which the particle density increases at a constant rate.

12:39PM W14.00008 Local Rearrangements in a Dense Granular Medium During Steady and Oscillatory Shear STEVEN SLOBOTBACK, University of Maryland: College Park, KRISZTIAN RONASZEgli, Budapest University of Technology and Economics, WIM VAN SAARLOOS, Leiden University, WOLFGANG LOSERT, University of Maryland College Park — Cooperative motion is a hallmark of dense granular media. Using the laser sheet scanning method described in [1], we are able to track the motions of all particles in a dense packing of spheres in three dimensions. We analyze the motions of all particles within a split bottom shear cell. We study both steady and oscillatory shearing processes. We compare relative motions of neighboring particles using a measure, P(cos(α)), based on a measure originally used by Ellenbroek et al [1]. The angle, α, is the angle between the relative displacements of neighboring particles and their bond vectors. A pair of neighboring particles where cos(α)=0 is called a rolling contact. We find that particles in contact tend to roll past one another, which is consistent with the findings made by Ellenbroek et al for systems close to jamming and we also find that the number of rolling contacts drops at the onset of a shear reversal. [1] Ellenbroek et al, to appear in Phys Rev Lett [2] Ellenboek et al., Phys Rev Lett, 97 258001 (2006)

12:51PM W14.00009 Three-dimensional Order and Self-Diffusion in a Cyclically Sheared Granular System ANDREAEA PANAITEscu, ARSHAD KUDROLLI, Physics Department, Clark University — We investigate the structure and dynamics of a dense granular packing (consisting of one millimeter diameter spherical glass beads) undergoing cyclic shear flow obtained by smoothly deforming a parallellepped shaped cell. Using a fluorescent refractive index matched particle tracking technique, we obtain the three dimensional position of particles in the central region of the shear cell as a function of shear cycle. The granular packing is observed to evolve towards crystallization over thousands of shear cycles and the packing fraction is correspondingly observed to increase smoothly from loose packing fraction. We obtain the Voronoi cell volume distributions from the measured positions, and compare them with various models which predict a Gamma-distribution and help us define a regularity factor. Further, we discuss the measured radial distribution and the bond-order parameter Q6 which are widely used to quantify local order in spherical particle systems. We find that the initial self-diffusion of the particles is anisotropic with diffusion greater in the flow direction compared with the velocity gradient direction which in turn is greater than the vorticity direction.

1:03PM W14.00010 Dynamic effective mass of granular media DAVID JOHNSON, Schlumberger-Doll Research, ROHIT INGAL, JOHN VALENZA, CHAUR-JIAN HSU, NICOLAS GLAND, HERNAN MAKSE, SCHLUMBERGER-DOLL RESEARCH COLLABORATION, LEVICH INST. COLLABORATION — We report an experimental and theoretical investigation of the frequency-dependent effective mass, M(ω), of loose granular particles which occupy a rigid cavity to a filling fraction of 48%, the remaining volume being air of differing humidities. We demonstrate that this is a sensitive and direct way to measure those properties of the granular medium that are the cause of the changes in acoustic properties of structures containing grain-filled cavities. Specifically, we apply this understanding to the case of the flexural resonances of a rectangular bar with a grain-filled cavity within it. The dominant features of M(ω) are a sharp resonance and a broad background, which we analyze within the context of simple models. We find that: a) These systems may be understood in terms of a height-dependent and diameter-dependent effective sound speed (∼ 130 m/s) and an effective viscosity (∼ 2 × 10^4 Poise). b) The effective acoustic Janssen effect in the sense that, at any frequency, and depending on the method of sample preparation, approximately one-half of the effective mass is borne by the side walls of the cavity and one-half by the bottom. c) On a fundamental level, dissipation is dominated by adsorbed films of water at grain-grain contacts in our experiments.

1:15PM W14.00011 ABSTRACT WITHDRAWN —

1:27PM W14.00012 Visualization of displacement fields in sheared granular systems KINGA LORINCZ, PETER SCHALL, University of Amsterdam — The jamming transition, i.e. the transition in a granular system from rest to flow is a fundamental problem of great importance to the understanding of a wide class of disordered materials: grains, clay and glassy materials such as molecular glasses and gels. We visualize the particles in a sheared three-dimensional granular packing immersed in an index matching liquid using confocal microscopy and laser sheet imaging. These experimental methods allow for an accurate determination of the displacement field of the particles at the onset of flow.


11:15AM W15.00001 Assembly and melting of DNA nanotubes and tile lattices THOMAS SOBEY, STEPHAN RENNER, FRIEDRICH SIMMEL, Biomolecular Systems und Bioelectronics, Physics Department E14, Technical University Munich, 85748 Garching, Germany — Programmable molecular self-assembly using DNA is allowing the demonstration of increasingly novel nanoscale structures such as lattices and tiles. Understanding the assembly and melting pathways of these will allow us to develop more complex and/or stable structures, and potentially useful nanomaterials. We experimentally show differences in these pathways by correlating temperature-controlled UV absorption measurements with atomic force microscopy, fluorescence microscopy, and transmission electron microscopy measurements. The three-dimensional nanotubes assemble in several hierarchical steps but melt in a single step, and this contrast is proposed to arise from the fundamental distinction between three-dimensional closed tubes and two-dimensional open lattices.
11:27AM W15.00002 Response of a self-assembling to mechanical stress. YVES DUBIEF, University of Vermont, Mechanical Engineering and Material Science Program, ROSS PACKARD, University of Vermont, Material Science program, SREEDHAR MANCHU, LEONIE COWLEY, University of Vermont, Mechanical Engineering Program — Coarse-grained molecular dynamics is used to characterize the mechanical properties of a solution of phospholipids and polyelectrolytes under shear and compression. DPPC (1,2-Dipalmitoylphosphatidylcholine) and polyelectrolytes are coarse-grained using the MARTINI force field. Simulations are performed using both GROMACS and LAMMPS. In our simulation, the solution is confined by two rigid walls. The objective of this work is to study the influence of the electrostatic nature of the wall on the self-assembling structure of the solution and to define the rheological and structural response of the solution under shear and compression by moving one wall.

1The computational support of the Vermont Advanced Computing Center is gratefully acknowledged. Y. Dubief and S. Manchu also thank Vermont Epscor and NSF for their support.

11:39AM W15.00003 Self-assembling structures resulting from the presence of polyelectrolytes in a solution of phospholipids. ROSS PACKARD, YVES DUBIEF. University of Vermont — The objective of this study is the characterization of self-assembled structures formed by the combination of phospholipids and polyelectrolytes. Coarse-grained molecular dynamics is used to simulate solutions of DPPC (1,2-Dipalmitoylphosphatidylcholine) and polyelectrolytes in a three-dimensional domain. The MARTINI database defines the topology of coarse-grained macromolecules and water, and simulations are performed using GROMACS. The interaction between negatively charged polyelectrolytes and positively charged hydrophilic heads of DPPC causes the disruption of lipid bilayer membranes and vesicles. The study attempts to define the conditions necessary for the formation of vesicles or organized networks of lipid bilayers that encapsulate the polyelectrolytes. Such structures are expected to play an important role in biological fluids subject to large mechanical stress.

1The computational support of the Vermont Advanced Computing Center is gratefully acknowledged.

11:51AM W15.00004 Self-organized Gels in DNA/F-Actin mixtures without Crosslinkers. JOHN BUTLER, GHEE HWEI LAI, OLENA Z RBI, University of Illinois at Urbana-Champaign, IVAN SMALYUKH, University of Colorado at Boulder, THOMAS ANGELINI, Havard University, KIRSTIN PURDY, University of Illinois at Urbana-Champaign, RAMIN GOLESTANIAN, University of Sheffield, GERARD C. L. WONG, University of Illinois at Urbana-Champaign — Interactions between flexible chains and rigid rods govern a broad range of soft matter systems. As a model system of like-charged rigid rods and flexible chains, we examine mixtures of DNA and filamentous actin (F-actin). Confocal microscopy reveals the formation of elongated nematic F-actin domains reticulated via defect-free vertices into a network embedded in a mesh of random DNA. Synchrotron small-angle x-ray scattering (SAXS) indicates that the DNA mesh squeezes the F-actin domains into a nematic state with an inter-actin spacing that decreases with increasing DNA concentration. Salt strongly influences the domain sizes and transitions the system from a counterion-controlled regime to a depletion-controlled regime. Both mechanisms of which are entropic in origin.

12:03PM W15.00005 Modeling the hydrophobic effect by coupling solutes to a lattice gas. AMISH PATEL, DAVID CHANDLER, University of California, Berkeley — In problems of biological assembly, manifestation of the hydrophobic effect is complex depending on the size as well as the conformation of the solute. The solute disrupts the inherent structure of the solvent by causing an unbalancing of attractive interactions experienced by the solvent molecules. The extent of this disruption determines the relative ease with which the solute is solvated. The theory of Lucio, Chait, and Chandler (LCW) successfully describes this rich interplay between the solute and solvent structures by coarse-graining the solvent density and analytically integrating out solvent fluctuations on a length scale smaller than the coarse-graining length ($L_c$). Since the implementation of LCW theory can be computationally very demanding the coarse-grained solvent density was mapped onto a lattice gas by ten Wolde, Sun and Chandler. In this work, we further improve upon the theory by relaxing certain assumptions about the unbalancing of attractive interactions on length scales smaller than $L_c$. In addition to a brief overview of the theory, results obtained by application of the theory to several pertinent problems of hydrophobic assembly will be presented.

12:15PM W15.00006 Direct Measurement of Inter-filament Forces in Neurofilament Networks: Synchrotron X-ray Diffraction Study under Osmotic Pressure. R. BECK, J. DEEK, C.R. SAPINYA, UC Santa-Barbara — Neurofilaments (NFs) are the major protein constituents in neuronal processes (axons and dendrites) that impart mechanical stability and act as structural scaffolds. The filaments assemble from different subunit proteins (NF-L, NF-M, NF-H) to form a 10 nm diameter flexible polymer with radiating unstructured sidearms. Recent work showed that at high protein concentration, the NFs form a nematic hydrogel network with a well-defined interfilament spacing as can be measured by synchrotron small-angle x-ray scattering (SAXS) [1]. In order to directly elucidate the interfilament forces responsible for the mechanical properties of NFs hydrogel, we conducted a SAXS-osmotic study, which yielded pressure-distance curves at different subunit compositions and monovalent salts. We show that filaments composed with NF-L and NF-M strongly attract each other through their polyampholyte sidearms, in particular at high monovalent salt. However, filaments comprised of NF-L and NF-H, show a distinctly different pressure-distance dependency, with much larger interfilament spacing and weaker salt dependence. Supported by DOE DE-FG-02-06ER46314, NIH GM-59288, NSF DMR-0803103, and the Human Frontier Science Program organization. [1] J.B. Jones, C.R. Sapinya, Biophys. J. 95, 823 (2008)

12:27PM W15.00007 Flexible ferromagnetic filaments and the interface with biology. ANDREJS CEBERS, MIHAIdsl BELSOVS, KASPARS ERGLIS, University of Latvia — Flexible ferromagnetic filaments exist in Nature (magnetotactic bacteria use them for the navigation purposes in the magnetic field of the Earth) and may be synthesized artificially by linking the functionalized ferromagnetic particles by DNA fragments of definite length. Ferromagnetic filaments allow to mimic self-propulsion of microorganisms by using AC magnetic fields. It is investigated both theoretically and experimentally. The elastic properties of the filaments are studied by kinetics of their orientation in an AC magnetic field of enough high frequency and allow to describe the observed deformation of the filaments at reversal of the magnetic field. By numerical analysis the Floquet coefficients for the dynamics of ferromagnetic filaments are calculated and the existence of stationary oscillations of U-like shapes is confirmed. These shapes self-propel perpendicularly to the AC magnetic field.

1Supported by grant Y2-ZP10-100 of University of Latvia.

12:39PM W15.00008 Electrokinetic effects near a membrane. DAVID LACOSTE, CNRS- Paris — We discuss the electrostatic and electrokinetic contribution to the elastic moduli of a cell or artificial membrane placed in an electrolyte and driven by a DC electric field. The field drives ion currents across the membrane, through specific channels, pumps or natural pores. In steady state, charges accumulate in the Debye layers close to the membrane, modifying the membrane elastic moduli. We first study a model of a membrane of zero thickness, later generalizing this treatment to allow for a finite thickness and finite dielectric constant. Our results clarify and extend the results presented in [D. Lacoste, M. Cosentino Lagomarsino, and J. F. Joanny, Europhys. Lett., 77, 18006 (2007)], by providing a physical explanation for a destabilizing term proportional to $k_{\text{p}}^3$ in the fluctuation spectrum, which we relate to a nonlinear ($E^2$) electro-kinetic effect called induced-charge electro-osmosis (ICEO). Recent studies of ICEO have focused on electrodes and polarizable particles, where an applied bulk field is perturbed by capacitive charging of the double layer and drives flow along the field axis toward surface protrusions; we predict similar ICEO flows around driven membranes, due to curvature-induced tangential fields within a non-equilibrium double layer, which hydrodynamically enhance protrusions.
12:51PM W15.00009 Piezoelectricity of Fluid Lipid Lamellar Phases and Their Chirality Dependence . JOHN HARDEN, NICHOLAS DIORIO, Kent State Univ., ALEXANDER PETROV, Institute of Solid State Physics, Bulgarian Academy of Sciences, ANTAL JAKLI, Liquid Crystal Institute, Kent State Univ. — The effects of chirality of membrane-forming lipids, has been largely ignored at present. Here we demonstrate that the chirality of phospholipids makes fluid lipid bilayers piezoelectric. This implies that chiral lipids would play a central role in the functioning of cell membranes as active mechano-transducers. By periodically shearing and compressing nonequilibrium lamellar phases of left (L-alpha-Phosphatidylcholine), right (D-alpha-Phosphatidylcholine) and racemic (DL-alpha-Phosphatidylcholine) lipids, we induced a tilt of the molecules with respect to the bilayer's normal and produced an electric current perpendicular to the tilt plane with the chiral lipids but not with a racemic mixture. This effect occurs because the lipids form a SmA† phase liquid crystal structure of the bilayers. Under molecular tilt, a ferroelectric SmC* phase is formed, creating a polarization which is normal to the tilt plane. This coupling allows for a wide variety of sensory possibilities of cell membranes such as mechano-reception, magneto-sensitivity, as well as in-plane proton membrane transport and related phenomena like ATP-synthesis, soft molecular machine performance, etc.

1:03PM W15.00010 Biomotor-functionalized Nanowires for Nanobio-mechanical Applications , DONG SHIN CHOI, NANO Systems Institute, Seoul National University, KYUNG-EUN BYUN, Department of Physics and Astronomy, Seoul National University, EUNHEE CHO, MOON-SOOK LEE, Samsung Electronics Co. Ltd., SEUNGHUN HONG, Department of Physics and Astronomy, Seoul National University — Protein motors such as actomyosin have shown the possibility as a building block for bio-inspired nanomechanical applications such as protein motor-based nanoscale engines. For such applications, it is crucial to combine protein motors with inorganic nanostructure such as nanowires. However, it has been difficult to functionalize nanowires/nanotubes with biological motors due to the incompatibility of such nanostructures with biomotors. Herein, we present a method to functionalize nanowires with biomotors while maintaining their functionalities. Significantly, we successfully demonstrated various motility assays using biomotor-functionalized nanowires, such as the delivery of nanowires functionalized with actin filaments on solid substrates.

1:15PM W15.00011 Non-monotonic mobility vs. length dependence observed in electrophoretic separation of 25 bp DNA ladder in Pluronic gels . SEUNGYONG YOU, DAVID VAN WINKLE, Department of Physics and Center for Materials Research and Technology, Florida State University — We electrophoresed a double-stranded DNA ladder first in an agarose gel, then in gels of Pluronic F-127 at room temperature. The DNA ladder consisted of 19 discrete fragments ranging in length from 25 to 450 bp at 25 bp increments plus 500 bp. The DNA fragments were first separated in agarose gel and stacked normally with 25 bp having the highest mobility. A single lane of the separated DNA ladder in the agarose gel was inserted at the edge of a Pluronic gel slab. The DNA was electrophoresed from the agarose into the Pluronic gels perpendicular to the original separation axis. Mobilities of DNA fragments increased from 25 bp to 175 bp and then decreased from 175 bp to 500 bp. The 25 bp and 500 bp bands of the ladder had approximately the same mobility in several different Pluronic gel concentrations. Both were slower than most bands in between. The highest mobility fragments with length of 175 bp have 99.5 nm contour length which is about 3.5 times the diameter of a micelle (17 nm). This result suggests a crossover from chromatographic separation to electrophoretic separation for these short DNAs. This research is supported by the state of Florida (Martech) and Research Corporation.

1:27PM W15.00012 Partition function and space-filling fractal-like networks of branching tubes, SAMIR LIPOVACA — We may think of the probability in quantum mechanics as a sort of fluid that flows from one point to another continuously and without loss or gain. We will utilize this fluid idea and imagine that probability flows through a space-filling fractal-like networks of branching tubes similar to the networks of a general model for the origin of allometric scaling laws in biology. In the general model, scaling laws arise from the interplay between physical and geometric constraints. This model provides a complete analysis of scaling relations for mammalian circulatory systems that are in agreement with data. We will show that there is a connection between a quantum system in thermal equilibrium and space-filling fractal-like networks. The relationship will be revealed through the calculation of the total fluid (probability) network volume. We will show that this total volume is proportional to the partition function of the related quantum system.

1:39PM W15.00013 The impact of conformational fluctuations on self-assembly: Cooperative aggregation of archael chaperonin proteins1, STEPHEN WHITEHAM, Lawrence Berkeley National Laboratory, CARL ROGERS, ANDREA PASQUA, UC Berkeley, CHAD PAAVOLA, JONATHAN TRENT, NASA Ames Research Center, PHILLIP GEISSLER, UC Berkeley — Protein complexes called rosettasomes self-assemble in solution to form large-scale filamentous and planar structures. The relative abundance of these aggregates varies abruptly with environmental conditions and sample composition. Our simulations of a model of patchy nanoparticles can reproduce this sharp crossover, but only if particles are allowed to switch between two internal states favoring different geometries of local binding. These results demonstrate how local conformational adaptivity can fundamentally influence the cooperativity of pattern-forming dynamics.

Thursday, March 19, 2009 11:15AM - 2:03PM — Session W16 DAMOP: Bosons in Optical Lattices I 317

11:15AM W16.00001 Generic Phase Diagram for Bose-Einstein Condensation of Weakly Interacting Symmetric Bosonic Mixtures, A.B. KUKLOV, CSI, CUNY, T. BLANCHARD, ENS, Cachan, France, B.V. SVISTUNOV, UMASS, Amherst, USA, and Kurchatov Institute, Russia — Weakly interacting Bose gas represents strongly correlated classical field within a domain (determined by the gas parameter ) of its Bose-Einstein condensation (BEC) temperature Tc. Thus, N-component weakly interacting mixtures representing some symmetry can potentially exhibit rich phase diagram (PD). In particular, it can feature quasi-molecular phases preceding actual formation of the ODRO in the vicinity of Tc. However, realization of a specific part of the PD depends on details of interactions. As examples, we consider mixtures characterized by O(2)×O(2) symmetry (N = 2) and spin S = 1 with the symmetry reduced to U(1)×U(1) (N = 3). Monte Carlo simulations of these systems find a single line of the respective two- and three-component BEC transitions which has tricritical point separating II and I order transitions. No quasi-molecular phases have been found despite that naive mean field (with one loop correction) predicts it. We discuss how such phases can emerge above the actual N-component BEC transition. One suggestion relies on Feshbach resonance detuned into negative inter-specie scattering length even when the gas parameter remains small. We acknowledge support from NSF grants PHY 0653153, 0653183 and CUNY grant 80209-0914.

3We acknowledge funding from the US Department of Energy and BioSim European Union Network of Excellence.
11:27AM W16.00002 Universal state diagrams for harmonically trapped bosons in optical lattices. MARCOS RIGOL, Georgetown University, GEORGE G. BATROUNI, INLN, Universite de Nice-Sophia Antipolis, VALERY G. ROUSSEAU, Institut-Lorentz Universiteit Leiden, RICHARD T. SCALETTA, University of California. Davis — We use quantum Monte-Carlo simulations to obtain universal zero temperature state diagrams for strongly correlated lattice bosons in one and two dimensions under the influence of a harmonic confining potential. Since harmonic traps generate a coexistence of superfluid and Mott insulating domains, we use local quantities like the quantum fluctuations of the density and a local compressibility to identify the phases present in the inhomogeneous density profiles. We emphasize the use of the ‘characteristic density’ to produce a universal state diagram which is relevant to experimental optical lattice systems, regardless of the number of bosons or trap curvature. We show that the critical value of $U/t$ at which Mott insulating domains appear in the trap depends on the filling in the system, and it is in general greater than the value in the homogeneous system. Recent experimental results by Spielman et al. [Phys. Rev. Lett. 100, 120402 (2008)] are analyzed in the context of our two-dimensional state diagram, and shown to exhibit a value for the critical point in good agreement with simulations.

11:39AM W16.00003 Occupation Statistics of a Bose-Einstein Condensate in a Driven Double Well Potential. K. SMITH-MANNSSCHOTT, Wesleyan University, Middletown, CT; MPI for Dynamics and Self-Organization, Goettingen, Germany, M. CHUCHEM, Ben-Gurion University, Beer-Sheva, Israel, M. HILLER, Physikalisches Institut, Albert-Ludwigs-Universitaet, Hermann-Herder-Str. 3, Germany, T. KOTTOS, Wesleyan University, Middletown, CT; MPI for Dynamics and Self-Organization, Goettingen, Germany, D. COHEN, Ben-Gurion University, Beer-Sheva, Israel — We consider the occupation statistics $P_i(n)$ of a Bose-Einstein condensate consisting of $N$ particles loaded in a double-well trap with intersite coupling $K$. Two dynamical scenarios are investigated: a) wavepacket dynamics and b) linear variation of the bias between the onsite energies of the two wells. In the latter case, we resolve three different behaviors as we increase the driving rate for intermediate values of the interatomic interaction $K/N < U < NK$: quantum adiabatic, diabatic, and sudden regime. We find that during the adiabatic to diabatic crossover, many-body Landau-Zener transitions play a dominant role, resulting in oscillations of the second moment of the occupation statistics. In contrast, the crossover to the sudden regime is characterized by a broad distribution $P_i(t \to \infty)$ which is reflected in a global maximum of the second moment.

1Supported by grants from the BSF and the DFG FOR760.

11:51AM W16.00004 Supersolidity of Cold Atomic Bose-Fermi mixtures in optical lattices. PETER P. ORTH, DORON L. BERGMAN, KARYN LE HUR, Yale University — An important possible mechanism for boson supersolidity in a Bose-Fermi mixture is the existence of a nested Fermi surface. Fermions then tend to exhibit a density wave at the nesting wavevector and imprint this order via boson-fermion interactions onto the bosons, which already support superfluidity. This coexistence of bosonic superfluidity and density wave order is a signature of the supersolid phase. We present new results concerning a cold mixture confined to a triangular optical lattice. For a fermionic density of $n_f = 3/4$ per lattice site, the Fermi surface exhibits both a van-Hove singularity and nesting. With a Landau-Ginzburg and a microscopic mean-field analysis, we predict the supersolid parametric regime in current experimental realizations of Bose-Fermi mixtures, and make comparisons with the square lattice geometry. We also discuss competing low-temperature phases such as a phase separated and a Mott insulating regime. Finally, we consider the case of spatially anisotropic hopping, which allows us to explore a quasi 1d regime of supersolidity.

12:03PM W16.00005 Magnetic phases of two-component lattice bosons at nonzero temperature. STEPHEN POWELL, University of Oxford — The realization of magnetically-ordered phases in optical lattices is set to be one of the next major experimental advances in the field of ultracold atoms. In the limit of strong repulsion and weak tunneling between lattice sites, perturbation theory predicts that two-component fermions form a Néel state with a two-sublattice structure, while bosons will tend to form a ferromagnetic insulator. This perturbative approach is, however, ill-suited for describing the physics above zero temperature and away from the strong-coupling limit. Here we address the phase diagram of two-component bosons at nonzero temperature using an approach that takes as its basis the standard mean-field theory for spinless bosons. This allows spin and charge excitations to be treated on an equal footing, and elucidates the competition between the possible magnetic and superfluid orders in the lattice.

12:15PM W16.00006 Ground State Phase Diagram of the Two-Component Bose-Hubbard Model. SEBNEM GUNES SOYLER, Department of Physics, University of Massachusetts, Amherst, BARBARA CAPOGROSSO-SANSONE, Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center of Astrophysics, NIKOLAY PROKOF’EV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, Amherst — We have performed path integral Monte Carlo simulations of the two-component hard-core Bose-Hubbard model on a square lattice at half-integral filling factor for each component. This system can be realized experimentally with heteronuclear bosonic mixtures in optical lattices with tunable interspecies interactions. Our results disagree with preexisting analytical treatments both quantitatively and qualitatively. We reveal the existence of an additional solid-superfluid phase for strong anisotropy between the hopping amplitudes which radically changes the topology of the ground-state phase diagram. The new phase is a direct consequence of effective interactions between “heavy” atoms mediated by the “light” superfluid component. Remarkably, mediated interactions are sign-alternating and thus lead to a rich variety of yet to be discovered quantum phases.

12:27PM W16.00007 Counterflow and paired superfluidity in one-dimensional Bose mixtures. ANZI HU, LUDWIG MATHEY, Joint Quantum Institute, University of Maryland and National Institute of Standard and Technology, Gaithersburg, MD 20899, IPPEI DANSHITA, Department of Physics, Faculty of Science, Tokyo University of Science, Shinjuku-ku, Tokyo 162-8601, Japan, CARL WILLIAMS, CHARLES CLARK, Joint Quantum Institute, University of Maryland and National Institute of Standard and Technology, Gaithersburg, MD 20899 — Experimental progress in recent years has made it possible to realize mixtures of cold atoms in optical lattices. In this talk, we present our work on two types of superfluidity in 1D Bose mixtures: the counterflow superfluid and the paired superfluid phase, each of which can coexist with charge-density wave order. We predict and identify these phases both with Luttinger liquid theory and with numerical simulations. Specifically, we show the phase diagram as a function of the filling fraction and the inter-species interaction. We address the question of realizability and detectability of these phases by adding a trap potential, and by calculating various quantities that can be measured in experiment.

12:39PM W16.00008 Determination of mixing or demixing state of a two-component BEC system. CHAO-CHUN HUANG, W. C. WU, National Taiwan Normal University — In a stable ultracold trapped two-component BEC system, it is shown that the condition $U_{12}U_{22} - U_{12}^2 > 0$ holds as long as the intra-species s-wave interactions $g_{11}$ and $g_{22}$ are both repulsive. Here $U_{ij} = g_{ij} \int |\Psi_i(r)|^2|\Psi_j(r)|^2$ with $\Psi_i(r)$ the wave function of species $i$. The condition is valid no matter the system is in a single-trap or in an optical lattice. Based on the variational approach, the condition has been applied to determine whether the system is in mixing or demixing state, both for the single-trap and optical-lattice cases. Phonon modes of the optical-lattice system are also shown to be intimately related to the above condition.

1Research supported by NSC, Taiwan.
11:51AM W17.00001 Time dependent DMRG for spectral functions of Heisenberg chains
STEVEN WHITE, UC Irvine, IAN AFFLECK, University of British Columbia, RODRIGO PEREIRA, UC Santa Barbara — Recently developed real-time DMRG techniques allow the calculation of space and time dependent spin-spin correlation functions for spin chain systems. These correlation functions can be Fourier transformed to obtain momentum and frequency dependent spectral functions. The growth of entanglement in the simulation as a function of time prevents us from performing the calculation for long enough times. We have found that the long time behavior can be extrapolated using either of two different techniques, allowing us to obtain very high resolution spectra with very high accuracy. We demonstrate these techniques for the S=1/2 Heisenberg chain and the XXZ S=1/2 chain.

We thank NCSA for supercomputer times.
11:27AM W17.00002 High-threshold surface code quantum computing: threshold calculation¹
, PETER GROSZKOWSKI, AUSTIN FOWLER, Institute for Quantum Computing, University of Waterloo, ASHLEY M. STEPHENS, University of Melbourne — Surface codes are topological quantum error correcting codes. In such codes, information is encoded in a collection of physical qubits arranged on a lattice, with only nearest-neighbor interaction required for processing and readout. In this talk we present a detailed account of a numerical threshold calculation for a planar surface code with boundaries (arXiv:0803.0272). In the end we find a threshold value that’s approaching 1%.

1NSERC

11:39AM W17.00003 Error threshold in topological quantum-computing models with color codes
, HELMUT KATZGRABER, ETH Zurich, HECTOR BOMBIN, MIGUEL A. MARTIN-DELGADO, Departamento de Fisica Teorica I, Facultad de Ciencias Fisicas, Universidad Complutense de Madrid, Spain — Dealing with errors in quantum computing systems is possibly one of the hardest tasks when attempting to realize physical devices. By encoding the qubits in topological properties of a system, an inherent protection of the quantum states can be achieved. Traditional topologically-protected approaches are based on the braiding of quasiparticles. Recently, a braid-less implementation using brane-net condensates in 3-colexes has been proposed. In 2D it allows the transversal implementation of the whole Clifford group of quantum gates. In this work, we compute the error threshold for this topologically-protected quantum computing system in 2D, by means of mapping its error correction process onto a random 3-body Ising model on a triangular lattice. Errors manifest themselves as random perturbation of the plaquette interaction terms thus introducing frustration. Our results from Monte Carlo simulations suggest that these topological color codes are similarly robust to perturbations as the toric codes. Furthermore, they provide more computational capabilities and the possibility of having more qubits encoded in the quantum memory.

11:51AM W17.00004 Performing measurement based quantum computation on ground states¹
, ANDREW DOHERTY, University of Queensland, STEPHEN BARTLETT, University of Sydney — One of the most exciting developments in quantum computing in recent years has been the realisation that there exist states of quantum many-body systems that can serve as a universal resource for quantum computing, where computation proceeds solely through single-qubit measurements. Although currently only a few isolated examples of such universal resource states are known, we discuss the possibility that there exist models of interacting spin systems in which an ordered phase is characterized by the ability to perform measurement-based quantum computation (MBQC). To identify such phases, we propose to use nonlocal correlation functions that quantify the fidelity of quantum gates performed between well separated qubits. The quantum computing phase is then characterized by set of order parameters corresponding to a universal set of quantum gates. We investigate a simple spin-lattice system based on the cluster-state model for MBQC by using a series of dualities with better studied models. We demonstrate that the model possesses a zero temperature phase transition between a disordered phase and an ordered “cluster phase” in which it is possible to perform a large class of one and two qubit quantum gates.

¹Supported by the Australian Research Council.

12:03PM W17.00005 Operator Theoretic Quantum Fault Tolerance¹
, GERALD GILBERT, YAakov S. WEINSTEIN, MITRE Quantum Information Science Group, VANEET AGGARWAL, Dept. of Electrical Engineering, Princeton University, A. ROBERT CALDER-BANK, Depts. of Mathematics and Electrical Engineering, Princeton University — We outline the advantages of an operator approach to quantum fault tolerance. Operator quantum fault tolerance is based on an explicitly stated halting condition, exact solutions of quantum error correction code dynamics, and as accurate and realistic descriptions as possible of the error models. This allows the proper integration of error correction and concatenation strategies with the system dynamics so as to better allocate quantum computational resources such as qubits, quantum gates, and computation time for quantum circuit design. We demonstrate these characteristics of the operator approach with an example of an asymmetric error model.

¹GG and YSW acknowledge support from the MITRE Technology Program; VA and ARC acknowledge partial support from the National Science Foundation and Air Force Office of Scientific Research

12:15PM W17.00006 Parallel Environment for Quantum Computing¹
, FRANK TABAKIN, University of Pittsburgh, BRUNO JULIA DIAZ, Universitat de Barcelona — To facilitate numerical study of noise and decoherence in QC algorithms, and of the efficacy of error correction schemes, we have developed a Fortran 90 quantum computer simulator with parallel processing capabilities. It permits rapid evaluation of quantum algorithms for a large number of qubits and for various “noise” scenarios. State vectors are distributed over many processors, to employ a large number of qubits. Parallel processing is implemented by the Message-Passing Interface protocol. A description of how to spread the wave function components over many processors, along with how to efficiently describe the action of general one- and two-qubit operators on these state vectors will be delineated.

¹Supported NSF and PSC Grants.

12:27PM W17.00007 Relation of operator Schmidt decomposition and CNOT complexity¹
, MARK COFFEY, RON DEIOTTE, Colorado School of Mines — We consider two-qubit operators and provide a correspondence between their Schmidt number and controlled-NOT (CNOT) complexity, where the CNOT complexity is up to local unitary operations [1]. The results are obtained by complementary means, and a number of examples are given. Additionally, we present results for exact decompositions of two-qubit operators in terms of CNOT [2]. Instances of these results are applicable to superconducting-flux qubit and other systems. [1]M. W. Coffey and R. Deiotte, Quant. Info. Proc. 7, 117 (2008). [2]M. W. Coffey and R. Deiotte, preprint (2008).

¹Work was supported in part by Air Force contract number FA8750-06-1-0001.

12:39PM W17.00008 New Method for the Calculation of Qubit Decoherence in the Presence of 1/f Noise¹
, DONG ZHOU, ROBERT JOYNT, Physics Department, University of Wisconsin-Madison — We present a new mathematical method for the calculation of qubit decoherence subject to a broad range of colored noise. The time evolution of the qubit density matrix is governed by a non-Hermitian quasi-Hamiltonian, mapping the problem onto a system consisting of a spin-1 particle (the qubit) coupled to spin-1/2 particles (the fluctuators). The method gives non-perturbative results for the energy relaxation, free induction decay (FID) and spin echo pulse measurements. This extends the range of known results to strong coupling, beyond the range of validity of Redfield theory and the commonly-used Gaussian approximation. New functional forms are suggested to explain the recent experiments by Kakuyanagi (PRL 98, 047004 (2007)) and Yoshihara (PRL 97, 167001 (2006)) on qubit decoherence with 1/f noise.

¹Support: NSF-DMR-0325634.
12:03PM W18.00003 Velocity Dependency of Dragging Force and Wetting Properties of High Viscous Liquids Using Constant Diameter Nanoneedle-Tipped AFM Probes, MEHDI YAZDANPANAH, ElectroOptics Research Institute and Nanotechnology Center, University of Louisville, MAHDI HOSSEINI, SANTOSH PABBA, CHARLES WALTER, JAYAN HEWAPARAKRAMA, ROBERT COHN, ELECTROOPTICS RESEARCH INSTITUTE AND NANOTECHNOLOGY CENTER, UNIVERSITY OF LOUISVILLE TEAM — A high aspect ratio and constant diameter Ag₂Ga nanoneedle grown on an AFM cantilever was used to perform F-D experiments on four different molecular weights of PDMS surfaces. The needle is partially inserted into and retracted from the liquid surface in various scan speeds. The viscous drag force causes the cantilever to deflect and recorded as a function of vertical displacement of the needle for each scan speed. The viscosity of the liquid is calculated by fitting a model into experimental data. The results show that the viscosity has strong correlation with the scan speed. Due to simple geometry of the needles, F-D curves are also interpreted to study the wetting properties (i.e. dynamic contact angle, meniscus height) of the PDMS at different scan speeds. Also, F-D curves are interpreted for polymer fiber formation during the capillary thinning and meniscus stretching that shown a strong correlation between the fiber length and the stretching velocity.

12:15PM W18.00004 Mechanical Properties of Individual Microparticle , SARA HASHMI, ERIC DUFRESNE, Yale University — Microparticles are important materials for both basic science and engineering and have wide applications from the study of phase transitions to the delivery of drugs. The method for the preparation of monodisperse polymeric micro particles, that is dependent on high angle x-ray scattering (HAXS) and magnetic resonance imaging (MRI), has been developed. The Brownian motion of the microparticles in liquids was measured using a high-speed synchrotron x-ray system. The size and shape of the microparticles were determined by high resolution x-ray microscopy. The mechanical properties of the particles were studied using atomic force microscopy (AFM) and small angle neutron scattering (SANS). The mechanical properties of the microparticles were found to be dependent on the size and shape of the particles. The results of this study will be useful for the design and development of microparticle-based drug delivery systems.

12:27PM W18.00005 Intrinsically Disordered Titin PEVK as a Molecular Velcro: Salt-Bridge Dynamics and Elasticity , JEFFREY FORBES, WANXIA TSAI, NIAMS/NIH, RICHARD WITTEBORT, Univ. of Louisville, KUAN WANG, NIAMS/NIH — Titin is a giant modular protein (3-4 MDa) found in the muscle sarcomere, where the intrinsically disordered and elastic PEVK segment plays a major role in the passive tension of skeletal and heart tissues. We have proposed that salt-bridges play a central role in the elasticity of PEVK. The 50 kDa engineered PEVK polypeptide shows well-resolved NMR spectra at all concentrations. From long-range NOE’s, we observed stable K to E salt-bridges. Simulated annealing with NMR restraints yielded a manifold of structures for an exon 172 trimer. Steered molecular dynamics simulations were done to study how the manifold of salt-bridges evolves during the stretching experiment. Repeated SMD simulations at slow velocity (0.0005 nm/ps) showed force spectra consistent with experimental AFM for force experiments on the polypeptide. SMD shows that salt-bridges occur even at high degrees of stretch and that these short range interactions are in integral part of the mechanical properties of PEVK. We propose that the long-range, non-stereospecific nature of electrostatic interactions provide a facile mechanism to tether and untether the flexible chains, which is important to maintain the accessibility of protein-protein interaction to these nanogel-like proteins.

12:39PM W18.00006 Mechanical Signal Filtering by Viscoelastic Properties of Cuticle in a Wandering Spider , MICHAEL E. MCCONNEY, Georgia Institute of Technology, CLEMENS SCHABER, University of Vienna, MICHAEL JULIAN, California State University Stanislaus, JOSEPH A.C. HUMPHREY, University of Virginia, FRIEDRICH BARTH, University of Vienna, VLADIMIR V. TSUKRUK, Georgia Institute of Technology — As recently found, in mecha-sensors of wandering spiders (Cupiennius salei) viscoelastic materials are important in signal filtering. We used atomic force microscopy to probe the time dependent mechanical behavior of these materials in five animals. We measured Young’s modulus of the cuticle during the stretching experiment. Simulated annealing with NMR restraints yielded a manifold of structures for an exon 172 trimer. Steered molecular dynamics simulations were done to study how the manifold of salt-bridges evolves during the stretching experiment. Repeated SMD simulations at slow velocity (0.0005 nm/ps) showed force spectra consistent with experimental AFM for force experiments on the polypeptide. SMD shows that salt-bridges occur even at high degrees of stretch and that these short range interactions are in integral part of the mechanical properties of PEVK. We propose that the long-range, non-stereospecific nature of electrostatic interactions provide a facile mechanism to tether and untether the flexible chains, which is important to maintain the accessibility of protein-protein interaction to these nanogel-like proteins.

12:51PM W18.00007 Bacterial Cell Wall Peptidoglycan at Single Molecule Resolution , AHMED TOHAMI, University of Guelph, MANFRED JERICHOW, Dalhousie University, VALERIO MATIAS, Max Planck Institute, ANTHONY CLARKE, TERRY BEVERIDGE, JOHN DUTCHER, University of Guelph — The major structural component of bacterial cell walls is the peptidoglycan sacculus, which is one of nature’s strongest and largest macromolecules that maintains the large internal pressure within the cell while allowing the transport of molecules into and out of the cell and cell growth. The three-dimensional structure of this unique biopolymer is controversial, and two models have been proposed: the planar model, in which the glycan strands lie in the plane of the cell wall, and the wall model, in which the glycan strands lie perpendicular to the cell wall. We have used atomic force microscopy to investigate the high resolution structure of isolated, intact sacculi of Escherichia coli K12 bacteria. Atomic force microscopy single molecule force spectroscopy was performed on single sacculi exposed to the tAmiB enzyme which cleaves the peptide-glycan bonds. Surprisingly, the measurements revealed individual strands of up to 250 nm in length. This finding combined with high resolution AFM images recorded on hydrated sacculi provide evidence for the validity of the planar model for the peptidoglycan structure in Gram-negative bacteria.

1:03PM W18.00008 Unfolding polyelectrolytes in a strong DC electric field, HSIAO, KUN-MAO WU, Department of Engineering and System Science, National Tsing Hua University — The behavior of single polyelectrolytes in multivalent salt solutions under the action of an electric field is investigated by computer simulations. The variation of chain size against the strength of electric field displays a sigmoidal transition, which defines a critical field. Above the critical field, the chain is unfolded into a rodlike structure, aligned parallel to the field direction. We show that the electric field induces a significant decrease in stiffness of the cuticular material and therefore less efficient energy transmission due to viscoelastic effects, as the frequency dropped to around 10 Hz. The stimulus transmitting cuticular material is acting as a high-pass filter for the mechanical stimulus on its way to the strain receptors. The results of this study indicate that viscoelastic mechanical signal filtering is an important tool for arthropods to specifically respond to biologically relevant stimulus patterns.

1:15PM W18.00009 Liquid Drop Pinning on Micro-patterned Surfaces , AHMED SOHIMAN, YEVGENI KALININ, ROBIN BAUR, ROBERT THORNE, LASSP, Cornell University — Pinning of liquid drops on surfaces is important in many areas of biotechnology. Micro-patterned surfaces provide a way to control drop pinning, and to investigate the mechanisms of pinning on rough (sucurface). Continuous circular rings on silicon wafers produced by etching the interior and surrounding silicon are shown to dramatically increase contact pinning. The critical apparent contact angle increases and the lifetime of the contact line is much longer and well correlated with parameters that describe the ring geometry, such as ring-wall height and width, as well as ring surface energy (hydrophilicity / hydrophobicity). Micro-patterns of surfaces in this way can be used to improve drop pinning, shape reproducibility and imaging in high-throughput protein crystallization.
Analytes, including cholesterol and ethanol. Higher enzyme loading, diffusion effects dominate. As a biosensing platform, the system also has the potential to be adapted to detect other biologically relevant analytes, including cholesterol and ethanol.

The authors deeply appreciate the help of Nan-Rong Chiou and the support from the NSF under IGERT (0221678) and NSEC (EEC-0425626).

1:39PM W18.00011 Patterning of Ferritin Nanoparticles on Gold Posts of Silicon Substrate

YUNXIA HU, DIAN CHEN, SOOJIN PARK, TODD EMRICK, THOMAS RUSSELL, Dept. of Polymer Science and Engineering, University of Massachusetts Amherst, HITACHI COLLABORATION — Patterning and immobilizing protein nanoparticles with nanometer-scale control has been proven integral to a range of applications in the development of biochip arrays, biosensor and electronic devices. Protein nanoparticles, such as ferritin nanoparticles, have a uniform size distribution and shape that can be used to construct well-defined patterns with nanoscale features. Here, the gold posts on silicon were produced using block copolymer PS (47.6 kg/mol)-b-P4VP (20.9 kg/mol) (PDI: 1.14) as a template and then gold chloride solution was loaded into P4VP domain. After reducing gold salt into gold and removing the block copolymer using an oxygen plasma, producing a pattern of gold posts. Thiol modified horse spleen ferritin are anchored to silicon substrate by the binding of thiol and gold. Scanning electron microscopy (SEM) shows that the feature size of gold posts decreased from 30 nm to 13 nm after attached with modified ferritin nanoparticles, which is consistent with size of modified ferritin. Also XPS result shows nitrogen and ion elements on ferritin-attached gold posts, and the signal of gold was attenuated after ferritin attached.

This work was supported by MURI, DOE, and MRSEC.

1:51PM W18.00012 Rapid Hydrogel Microactuator Using Elastic Instability

HOWN LEE, CHUNG-GUANG XIA, NICHOLAS FANG, University of Illinois at Urbana-Champaign — Rapid Hydrogel Microactuator Using Elastic Instability Inspired by rapid movement of sensitive plants such as Venus flytrap [1], we present an innovative way to enhance actuation speed of hydrogel micro devices by exploiting elastic instability. In this work, hydrogel micro devices in doubly curved shape are designed and fabricated using projection micro-stereolithography [2], with embedded microfluidic channels on the surface. Local swelling of hydrogel around channels causes bending which subsequently induces stretching of the soft structure. Such coupling gives rise to elastic instability, the onset of which triggers rapid conversion of stored elastic energy into kinetic energy in fast motion. We further designed a set of devices with different dimensions, which leads to different coupling of elastic energy in bending and stretching [1]. Our experimental results verified the critical coupling parameter that triggers snap-buckling motion. Ongoing experiments are investigating the actuation speed as a function of coupling parameter. This novel approach promises new potential applications for hydrogel based devices in various fields of study including microfluidics, soft robotics, artificial muscle, and drug delivery. Reference [1] Forstre, Y., et al, Nature, 433, 421-425 (2005) [2] Sun, C., et al, Sensors and Actuators A, 121:1, 113-120 (2005)

2:03PM W18.00013 Effect of Single Bacterium Cell and DNA Attachment on the Electrical Properties of Chemically Modified Graphene Sheets

NIHAR MOHANTY, VIKAS BERRY, Kansas State University — Chemically modified graphene (CMG) sheets are expected to have a considerably different electrical sensitivity to molecular attachment than the pristine graphene sheets. Here we present the electrical-interfacing properties of (a) CMG’s hybrids with single bacterial cells, (b) CMG with DNA (single and double stranded) tethered on graphene-surface and (c) CMG with polyelectrolyte-layer assembled on surface. These hybrids function as: (a) single bacterium devices, (b) DNA hybridization sensor and (c) charge polarity sensitive chemical-detector, respectively. A single bacterium attachment leads to generation of ~1400 holes on a CMG while hybridization of ~4 DNA molecules on graphene-DNA-carpets lead to generation of one hole. Further explanation of the attachment-potential, system-reversibility and sensitivity will also be presented.

Thursday, March 19, 2009 11:15AM - 2:15PM — Session W19 DPOLY: The Physics of Polymer Nanocomposites: Grafting and Dispersion

11:15AM W19.00001 A theoretical study of polymer grafted nanoparticles as fillers in polymer nanocomposites

ARTHI JAYARAMAN, University of Colorado-Boulder, KENNETH SCHWEIZER, University of Illinois-Urbana — We have generalized the microscopic Polymer Reference Interaction Site Model (PRISM) theory to study the structure and phase behavior of polymer-tethered spherical nanoparticles (fillers) in a homopolymer matrix. In the absence of a polymer matrix, melts of polymer-tethered nanoparticles show strong concentration fluctuations indicative of aggregate formation and/or a tendency for microphase separation as the total packing fraction and/or nanoparticle attraction strength increase. In the presence of a polymer matrix there is competition between nanoparticle attractions, steric repulsion between grafted polymers, and polymer matrix induced depletion-like attraction. For single tethered particles, volume of the tether being equal to the volume of the nanoparticle, the apparent microphase spindal curve exhibits both dilution-like and depletion-like features, and a non-monotonic dependence on matrix chain length. As the particle size and tether length are increased, such that the total space filling volume of the tether continues to equal the nanoparticle volume, the shape of the microphase spindal curve remains unchanged, but the effect of matrix polymer chain length on the spindal temperature diminishes. The effect of various parameters on the spindal temperature will be presented.

11:27AM W19.00002 Highly-branched anisotropic hybrid nanoparticles at surfaces

VLADIMIR TSUKRUK, Georgia Tech — We present a brief overview of our recent studies on combined hybrid anisotropic structures composed of inorganic nanoparticles and highly branched molecular such as modified silsesquioxanes polyhedra cores (POSS) with mixed hydrophobic-hydrophilic tails and silver nanowires with functionalized star block copolymer with embedded gold nanoparticles (nanocobs). We demonstrate two-stage melting of that branched POSS and their ability to form monolayer and multilayered LB structures. On the other hand, we observed that silver-BCP-gold nanocobs display extremely bright Raman scattering caused by surface enhanced Raman effect with very different longitudinal and transversal optical properties as revealed by high-resolution confocal Raman microscopy. To study these hybrid nanostructures we applied combined AFM, SEM, TEM, XPS, SERS, UV-vis, and XR techniques.
11:39AM W19.00003 Particle Dynamics within Self-Assembling Polymer-Grafted Spherical Nanoparticles, PINAR AKCORA, University of Missouri, SANAT K. KUMAR, Columbia University, YU LI, BRIAN BENICEWICZ, University of South Carolina, SURESH NARAYANAN, Argonne National Laboratory, COLUMBIA UNIVERSITY COLLABORATION, ARGONNE NATIONAL LABORATORY COLLABORATION — We have recently shown that the self-assembly of polymer grafted spherical nanoparticles can be achieved by varying the brush grafting density and chain length. The mechanical behavior of these nanocomposites with various states of particle dispersion has been explored using x-ray photon correlation spectroscopy. Nanoscale and macroscopic dynamic measurements show that mechanical reinforcement results from the percolated and also strongly entangled brushes forming strong networks. Particle dynamics within various polymeric nanostructures will be discussed.

11:51AM W19.00004 Thermally Stable Au Nanoparticles via Photo-crosslinkable Polymeric Stabilizers, JOONA BANG, MISANG YOO, Korea University, BUMJOON J. KIM, KAIST — Polymer nanocomposites consisting of polymers and inorganic nanoparticles (NPs) have attracted many interest due to their applications such as solar cell, sensors, catalysts and ferroelectric devices. To integrate NPs into polymer matrix in the controlled manner, thiol-terminated stabilizers have been used to tune the surface property of NPs such as Au, Pt, CdSe, etc. However, a practical use of such particles in the nanocomposites is very limited by thermal instability even at ~90 °C, leading to the agglomeration of NPs. To impart the thermal stability of NPs, we modified Au NPs surface using UV-crosslinkable polymeric stabilizers. After UV-crosslinking, it was found that the Au NPs exhibit the excellent stability at high temperature (~180 °C) in both solution and thin-film states. Furthermore, we demonstrate that thermally stable Au NPs can be used as compatibilizers in PS/PMMA blends. The NPs at the PS/PMMA interface produced the dramatic reduction in the droplet size after 1 day of thermal annealing at 180 °C, in which the particle size is unchanged.

12:03PM W19.00005 Design of Polymer-Grafted Particles for Biocompatibility, DAVID TROMBLY, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin — Drug designers often coat drug particles with grafted polymers in order to introduce a net repulsion between the particles and blood proteins. This net repulsion results from the energy cost of compressing grafted chains on approach of proteins. It thus overcomes the Van Der Waals attraction between drug and protein which would otherwise cause particle-protein agglomeration and ultimately thrombosis. This study proposes to develop a fundamental understanding of the role of different features in controlling the efficacy of the grafted layers. We address this issue by developing a framework to predict the interactions between a polymer-coated spherical particle and a bare spherical particle. In order to fully capture the two-sphere system, a numerical solution of polymer mean field theory is used in a bispheerical coordinate system. Results for protein-particle interaction energies for different design parameters will be presented. For biological applications, polyethylene glycol is often used as the grafted polymer. The unique properties of this molecule will be accounted for using the n-cluster model.

12:15PM W19.00006 Synthesis of Polystyrene-Silica Composite Particles via One-Step Nanoparticle-Stabilized Emulsion Polymerization, LENORE DAI, HUAN MA, Department of Chemical Engineering, Arizona State University — Polystyrene-silica core-shell composite particles are prepared by one-step emulsion polymerization with a nonionic initiator V.A.-086, solely stabilized by silica nanoparticles. The silica nanoparticles are successfully incorporated into the shell, likely due to the fact that the nanoparticles are thermodynamically favorable to self-assemble and remain at the liquid-liquid interfaces during the emulsion polymerization. The silica content, determined by thermogravimetric analysis, is approximately 20 wt.%. However, we further explore the polymerization mechanism by studying the particle growth as a function of initiator concentration and reaction time: when the silica/monomer ratio is increased from 0.83 without reaction time decreases for a fixed monomer amount, probably due to a larger number of nuclei at the initial stage of polymerization. Further increasing the initiator/monomer ratio to 4.2 wt.%, which may be limited by the stabilization provided by a fixed concentration of silica nanoparticles. The surface coverage also changes with initiator concentration and reaction time although the underlying mechanism is not fully understood.

12:27PM W19.00007 Effects of Grafted Chain Density on Nanoparticle and Melt Structure, JOSHUA KALB, SANAT KUMAR, Columbia University, ROBERT S. HOY, University of California, Santa Barbara, GARY S. GREST, Sandia National Laboratories — Applications of nanoparticles have increased dramatically over the last few years with uses ranging from scratch proof glass to lubricants to fighting cancer. Grafting polymer chains to these systems further increases the range of their properties, but still much remains to understand about the behavior of ‘brush grafted nanoparticle’ systems, particularly in their interaction and entanglement with a polymer melt. Previous works on polymer brushes attached to a flat surface have demonstrated that entanglements between the attached chains and the polymer melt depend strongly on coverage and length of the attached chains. Allowing for a curved grafted nanoparticle surface allows for a wider range of interactions with the melt. Here we present molecular dynamics simulations of the structure of grafted nanoparticles and their entanglements with a highly entangled melt. Individual entanglements are identified using a modified version of primitive path analysis.

12:39PM W19.00008 Polyethylene/organically-modified layered-silicate nanocomposites with antimicrobial activity, P. SONGTIPYA, M.M. JIMENEZ-GASCO, E. MANIAS, Departments of Materials Sci & Eng and Plant Pathology, Penn State University — Despite the very intensive research on polymer nanocomposites, the opportunities for new functionalities possible by nanofillers still remain largely unexplored. Here, we present polyethylene/organoclay nanocomposites that exhibit strongly enhanced mechanical performance and, at the same time, also an antimicrobial activity originating from the organo-filler nature. Specifically, PE/organically-modified layered-silicate nanocomposites were prepared via melt-processing, and antimicrobial activity was designed by proper choice of their organic modification. Their antimicrobial activity was measured against three microorganisms: Penicillium roqueforti and Penicillium claviforme, and Fusarium graminearum. We study the changes in the mechanical properties of the nanocomposites, the decrease in the percolation threshold from the single to the multi-layered silicate nanocomposites, and the enhancement of the mechanical performance of the organo-clay nanocomposites.

12:51PM W19.00009 Modeling of block copolymer/nanoparticle nano-composites, MARCO PINNA, University of Central Lancashire, Preston, UK, IGNACIO PAGONABARRAGA, University of Barcelona, Spain, ANDREI ZVELINDOVSKY, University of Central Lancashire, Preston, UK — We develop a coarse grained simulation technique to study dynamics in soft nano-composites. The system consists of block copolymer melt with embedded nano-size particles. The time evolution of the system is described by a hybrid method combining a field based simulation for block copolymer component and a particle based method for nano-colloids. The block copolymer is modelled by cell dynamics simulation technique, and nano-particles are modelled as soft particles with prescribed density profile. A cross interaction term is controlling the interplay of dynamics of both components. The influence of nano-particles on block copolymer morphology is investigated.
further insight into the factors that determines the conformation of the PPEs. We have shown that short alkyl PPEs are fully stretched out. With increasing molecular weights they assume a worm like configuration. The current study provides further understanding of this behavior by studying the conformation of PPEs in toluene solutions. Toluene is a good solvent for the backbone and a poor solvent for the substituting side chains. Small angle neutron studies (PPEs) polymers, electro-active polymers, in dilute toluene solutions. The conformation of PPEs determines the conjugation of the polymer and their assembly para-polyphenyleneethylenes, SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Laboratory — The interfacial region in polymer blends has been identified as a low viscosity region in which considerable slip can occur when the blend is subjected to shear forces. Here we use Molecular Dynamics simulations to establish the role that added nanoparticle fillers play in modifying the interfacial rheology. By choosing conditions under which the fillers are localized, either in the two phases or at the interface, we can look at the interplay between the decomposition of nanoparticles and the change in the interfacial slip behavior. We examine particle size, attraction between the particle and the polymer component, and the amount of filler in the material. Our studies are performed both above and below the point at which the filler particles form a transient network in the blend.

1:15PM W19.00011 Synthesis of composite polymer nanoparticles, EDWARD VAN KEUREN, MAKI NISHIDA, Georgetown University, Dept. of Physics — We have been developing composite nanoparticles using the reprecipitation method or miniumulsion polymerization. These methods enable the combination of multiple functional components, such as large metal or metal oxide clusters and molecular species such as fluorophores, into polymer nanoparticles. The incorporation of these into the polymer or monomer precursors requires a detailed understanding of the mutual solubility of the components. We present fluorescence correlation spectroscopy measurements of molecular solubility and results from dynamic light scattering, electron microscopy and Raman spectroscopy that reveal the morphology and composition of these particles.

1:27PM W19.00012 Relaxation behaviors of nanoparticles in polymer composites: influence of local frictions by polymer chains, BYEONGDU LEE, PAPPANANN THIYAGARAJAN, SURESH NARAYANAN, ALEC SANDY, VILAS POL, CHIEH-TSUNG LO, DAVID BOHNSACK, Argonne National Laboratory — The dynamics of Au nanoparticles (AuNP) tethered with thiol-terminated polystyrene (PS) in the composites with poly(styrene-b-2-vinylpyridine) diblock copolymers (PS-PVP) have been studied by x-ray photon correlation spectroscopy and small-angle x-ray scattering. Relaxation behaviors of nanoparticles located selectively in PS domain due to enthalpic interaction, interestingly, are not correlated with those of matrix polymer chains, i.e., their relaxation times are not dependent on the molecular weights of PS-PVP. They relax faster in PS-PVP than in PS homopolymer having the same molecular weight as the PS brush of PS-PVP. On the other hand, the influence of morphological structures of PS-PVP, however, is significant: AuNP moves faster in the lamellae phase than those in the cylinder phase.

1:39PM W19.00013 Nano-particle distribution in a polymer nano-composite, PANAGIOTIS MANIADIS, Theoretical Division and CNLS, Los Alamos National Lab, IOANNIS N. TSIMPANOGIANNIS, Environmental Research Laboratory, National Center for Scientific Research “Demokritos”, Greece, EDWARD M. KOBER, Institute of Multiscale Modeling and Simulations, Los Alamos National Lab, TURAB LOOKMAN, Theoretical Division, Los Alamos National Lab — We use the hybrid particle-Self Consistent Field calculation (hybrid particle-SCF) to study the distribution of particles in a multi-block copolymer nano-composite. Using the static approach, we first find the effective interaction potential between the nano-particles and the polymer. The interaction has an entropic and an enthalpic component. The dynamical simulation confirms that the distribution of particles has a maximum at the minima of the interaction potential. We also study the situation where the nano-particles are distributed in a blend of AB diblock and A homopolymer. In this case, for large homopolymer concentration (larger than 20%), an interface is created between components that are identical, but they come from different types of polymer chains (i.e. the AB diblock or the A homopolymer). We find that the interaction potential has a minimum in this A/A interface which is of pure entropic origin. Furthermore the dynamical simulation reveals that the distribution of nano-particles has a maximum in the area around this interface.

1:51PM W19.00014 Thermoresponsive Self-Assembling Nanocomposites, KARI THORKELSSON, YUE ZHAO, THOMAS SCHILLING, University of California, Berkeley, ALEXANDER MASTROIANNI, JOSEPH M. LUTHER, University of California, Berkeley, Lawrence Berkeley National Laboratory, YUE WU, University of California, Berkeley, A. PAUL ALIVISATOS, TING XU, University of California, Berkeley, Lawrence Berkeley National Laboratory — Nanoparticles have significant potential for use in fields including photovoltaics and memory storage, but to realize this potential, their distribution must be finely controlled. We present here a versatile method to achieve such control, using a diblock copolymer supramolecule composed of polystyrene-block-poly(4-vinylpyridine) (PS-b-P4VP) and 3-pentadecylphenol (PDP). The PDP hydrogen bonds to the P4VP block, forming a comb block. This change in morphology causes the PS-b-P4VP(PDP) supramolecule to force the nanoparticles into well-organized rows one nanoparticles thick at the center of the P4VP(PDP) domains. Furthermore, the morphology of the supramolecule-nanoparticle composite changes with temperature as hydrogen bonding is broken and the PDP becomes soluble in the PS block. This provides a useful path for the production of polymer-based thermoresponsive nanocomposites.

2:03PM W19.00015 Self-Assembly of Polymer-Decorated Nanoparticles in the Bulk and in a Nanometric Confined Region, DAMIEN MAILLARD, SANAT KUMAR, Department of Chemical Engineering, Columbia University, New York, NY, PINAR AKCORA, Department of Chemical Engineering, University of Missouri, Columbia, MO — As shown previously by simulation and TEM studies in the bulk, PS grafted nanoparticles when mixed a PS matrix self-assemble into a range of superstructures. These self-assembled structures can be regrouped into a phase diagram in which the leading parameters are the particles grafting density and the molecular weight ratio of the grafted and free matrix chains. Depending on those parameters the particles can be well dispersed or aggregated in a core-shell “onion” morphology or in one (strings), two (interconnected sheets) or three (spherical aggregates) dimensions. Here we consider the corresponding behavior in thin films (100 nm thick) using in-situ phase contrast AFM. In addition to yielding the morphologies, this protocol allows us directly visualize the aggregation process of the particles.


11:15AM W20.00001 Conformational Study of Di-Substituted para-polyphenyleneethylenes (PPE) in Dilute Solutions, SABINA MASKEY, FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Lab — Molecular dynamics (MD) simulations have been used to study the conformation of highly rigid di-substituted para-polyphenyleneethylenes (PPEs) polymers, electro-active polymers, in dilute toluene solutions. The conformation of PPEs determines the conjugation of the polymer and their assembly mode which in turn affect the electro-optical properties. In solution, the conformation is determined by molecular parameters including the length of the polymer and the nature of the side chain, coupled with the interaction of the molecules. The present study investigates the effects of molecular weight and the nature of the side chain in toluene solutions. Toluene is a good solvent for the backbone and a poor solvent for the substituting side chains. Small angle neutron studies have shown that short alkyl PPEs are fully stretched out. With increasing molecular weights they assume a worm like configuration. The current study provides further insight into the factors that determines the conformation of the PPEs.
11:27AM W20.00002 Crystal and Rotator Phases of n-alkanes: a Molecular Dynamics Study
NATHANIEL WENTZEL, SCOTT T. MILNER, Pennsylvania State University — The odd n-alkanes exhibit a wide variety of solid phase behavior; experimentally observed phases include an orthorhombic crystal phase, in which the molecules show long range herringbone order, and rotator phases in which the molecules do not diffuse but display various degrees of disorder. The rotator phases are of interest because they are implicated in the nucleation of n-alkane and polyethylene crystals. C_{23} has been found experimentally to have two stable rotator phases, orthorhombic R_{II} and hexagonal R_{I}, at temperatures between the crystal and melt. The crystal-R_{II} and R_{II}-R_{I} phase transitions have been observed to be weakly first order. Simulations of C_{23} to date have found the R_{II} phase but not the R_{I} phase, and have not much characterized the phases or the transitions between them. We report our results for local order and pretransitional fluctuations of rotator phases, from our all-atom molecular dynamics simulations of thin layers of C_{23}. We also comment on how these properties relate to the experimentally observed phase transitions.

11:39AM W20.00003 Computational Modeling of Polymers and the Influence of Molecular Level Structural Features on Mechanical Properties
THOMAS CLANCY, SARAH-JANE FRANKLAND, National Institute of Aerospace — The role of molecular structure on the mechanical properties of polymer based materials is investigated through atomistic based molecular dynamics simulations. Models of crosslinked polymers were built with a range of moisture content in order to study the effect of environmental exposure on mechanical properties. Another key structural parameter, the degree of crosslinking, was also varied. The molecular structural features associated with these parameters are studied for their influence on the mechanical properties. The relative motion of crosslink points and the influence of penetrants such as water are investigated under deformation conditions. The mobility of penetrants within the polymer matrix is studied under equilibrium and deformation conditions in order to assess the role of these structural features on the mechanical properties as well as to assess the influence of deformation on diffusion rates.

11:51AM W20.00004 Hydrogen Bonding Structure in Hyperbranched Aliphatic Polymers Studied by MD Simulations
BRIAN OLSON, MUKUL KAUSHIK, SERGEI NAZARENKO, University of Southern Mississippi — Hyperbranched aliphatic polymers based on dimethoxy propionic acid (bis-MPA) as the repeating unit and ethoxylated pentaoxythanol as the tetrafunctional core gained widespread attention due to their unusual structure and properties. These globular macromolecules possess a large number of hydroxyl functional groups in particular on their periphery. These hydroxyl groups interact readily through hydrogen bonding (HB) and form clusters responsible for many physical properties of this system. The structure of these clusters however remains unclear. Therefore MD simulations have been used to elucidate the structure of these clusters. MD simulations revealed that peripheral hydroxyl groups form linear hydrogen bond clusters (strings) similar to those proposed in hydrofluoric acid (HF) but considerably shorter consisting of 4-10 hydroxyl groups per cluster. Simulations also led to prediction of WAXS pattern for these hyperbranched polymers in the bulk with the characteristic peak at 2θ = 30° due to O-O correlations similar to those in water. The predictions were in excellent agreement with the experimental WAXS data.

12:03PM W20.00005 Phases of functionalized polymer-inorganic composites in solution studied via molecular dynamics
JOSHUA ANDERSON, RASTKO SKNEPNEK, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Using self-assembling polymer systems to direct the formation of inorganic crystals, polymer-inorganic composite materials offer new opportunities in materials design. Molecular dynamics simulations allow for an exploration of the wide range of phases in these systems. Amphiphilic ABA triblocks with A hydrophilic, B hydrophobic, and functional ends with an affinity to inorganic particles are modeled to capture the minimum physics needed to describe polymer-inorganic systems currently being investigated by experiment. A number of phases are formed in solution as the attraction strength between the inorganic particles and the affinity of those particles to the functional end beads of the polymer are varied. Some of the phases found include hexagonal, square columnar, lamellar, perforated lamellar, and the gyroid. Polymer stretching plays an important role in each of the phases found, with a characteristic multi-modal behavior in the polymer end to end distance distribution. In the gyroid phase, for instance, the peaks correspond to the polymers being in two preferred conformations: v-shaped with a small end to end distance and fully extended in a line with the largest possible end to end distance. At high interaction strengths, inorganic particles are found to crystallize and form plate-like structures.

12:15PM W20.00006 The effect of chain stiffness on the structure and phase behavior of diblock copolymer melts
G. LEUTY, MESFIN TSIGE, Southern Illinois University at Carbondale — In block copolymers the covalent bond joining the different immiscible block segments prevents the occurrence of macroscopic phase separation of the different components of a copolymer chain. Instead, the block segments give rise to well-organized periodic domain nanostructures whose size and shape mainly depend on the dimensions of the blocks and the segment-segment interaction parameters. Variations in the stiffness of the different block segments can directly affect the morphology of the system and may result in a very rich phase behavior. To the best of our knowledge, there is no theory at the atomic or molecular level that explains how variations in the stiffness of the different block segments can affect the dynamics and morphology of these systems. We have studied the microphase separation of symmetric diblock copolymers with variable block stiffness and different block chain length using coarse-grained molecular dynamics simulations. The morphology of the diblock systems we studied is found to be strongly dependent on the relative stiffness of the two block segments.

12:27PM W20.00007 Rigidity transition with increasing crosslinking of a single macromolecule
JIUJU LIU, PHILLIP DUXBURY, Michigan State University — A nano-particle can be formed by the intramolecular crosslinking of a polymer chain. In this process the rigidity of the system increases with the crosslinking density. We carried out extensive molecular dynamics simulations of the intramolecular crosslinking on six different models to study their rigidity transitions. It was found the crosslinking satisfiability of the system is greatly affected by its rigidity. A facile analysis of floppy modes of the system was employed to determine the rigidity transition threshold and a good agreement with simulation data was obtained.

12:39PM W20.00008 Spreading of Droplets on Viscous Polymer Liquids
FLINT PIERCE, DVORA PERAHIA, Clemson University, GARY GREST, Sandia National Laboratories — Significant strides have been made in understanding the spreading of liquid droplets on solid surfaces. However from biological complexes to polymeric interfaces, the surfaces are not ideal; explicitly, the surfaces may dynamically respond as spreading takes place and the droplets may partially penetrate. Molecular dynamic simulations were carried out to investigate the spreading of liquid droplets of short chains on films of viscous polymer melts. Unlike the spreading on solid surfaces, the droplets simultaneously spread and penetrate. The degree of penetration and the magnitude of damping from the film depend on the viscosity of the underlying liquid and the relative interaction of the two constituents. At the interface with viscous films a precursor foot spreads ahead of the droplet whereas on top of less viscous interfaces, the droplets penetrate while spreading with no precursor foot. A kinetic model described the spreading of shorter chain length droplets, while a hydrodynamic model better expresses the spreading of longer chain length liquid. Supported in part under DOE contract No. ER46456.
12:51PM W20.00009 Shear rate threshold for the onset of boundary slip in dense polymer films

Molecular dynamics simulations are carried out to investigate the dynamic behavior of the slip length in thin polymer films confined between atomically smooth surfaces. The polymer melt is modeled as a collection of bead-spring chains of 20 Lennard-Jones monomers interacting through the FENE potential. We found that at high melt densities and low shear rates the fluid velocity profiles acquire a pronounced curvature near the walls and the slip length is approximately equal to the thickness of the immobile boundary layer. The linearity of the fluid velocity profiles is restored at higher shear rates where the slip length increases rapidly as a function of shear rate. We will show that the friction coefficient at the interface between a polymer melt and a solid wall follows power law decay as a function of the slip velocity. At large slip velocities the friction coefficient is determined by the product of the value of surface induced peak in the structure factor and the contact density of the first fluid layer near the solid wall. A relation to recent slip flow experiments is discussed.

1 ACS Petroleum Research Fund

1:03PM W20.00010 Direct Numerical Evaluation of Plateau Modulus of Entangled Polymer Melts via Multi-Scale Molecular Dynamics (MD)

Plateau modulus and viscosity of entangled polymer melts can be calculated by off-diagonal elements of stress tensor, which are connected by the Green-Kubo relation and tube theory. However, direct numerical evaluation of plateau modulus via stress autocorrelation function (SAF) from MD simulation is a big challenge in a computational point of view due to the following reasons: strong fluctuations, long relaxation times and large spatial scales. In the present work, SAFs of entangled polymer melts are calculated by coarse-grained MD. We find that the use of time-averaged stress helps to reduce strong noise in SAF while capturing most local chain relaxations. Plateau values by SAF are compared with plateau values predicted from the entanglement length evaluated via primitive path analysis (PPA). The importance of well equilibrated melts for such an analysis is shortly discussed.

1:15PM W20.00011 Cole-Davidson Glassy Dynamics in Simple Chain Models

Cole-Davidson function was used to fit the response functions. For the systems studied, the Cole-Davidson function provided remarkably accurate fits (as compared to the transform of the Kohlrausch-Williams-Watts (KWW) function). The only appreciable deviations from the simulation results were in the high frequency limit and were due to ballistic, or free rotation, effects. The accuracy of the Cole-Davidson function appears to be the result of the transition in the time-domain from stretched exponential behavior at intermediate time to single exponential behavior at long time.

1:27PM W20.00012 Glass transition temperature of PIB, PDMS and PMMA from small-time simulations

Glass transition temperatures $T_g$ of poly(isobutylene), poly(dimethyl-siloxane), and poly(methyl methacrylate) from small-time atomistic molecular dynamics simulations. The different fragilities of these materials are reflected in the results of the simulations. One approach involved measurement of the apparent softening of the “cage” in which a monomer is bound, while another involved studying autocorrelation of a convolution of the velocity with a smoothing function in order to detect the frequency of escapes from the “cage.” To check the accuracy of the short-time methods, the $T_g$ of the polymers was also found using conventional diffusion simulations in which the rate of increase of the root mean squared displacement of an atom, monomer, or molecule is measured at very long times. The economical short-time simulations yielded results for $T_g$ that were identical to those of the computer-intensive long-time simulations.

Work supported by DOE Grant DE-FG02-05ER46244

1:39PM W20.00013 Translocation of a Polymer Through a Nanopore in the Presence of Obstacles

Translocation of a polymer through a nanopore is interesting both as a process of fundamental biological importance and as relevant to the development of next-generation DNA sequencing technology. Due to the time and length scale of typical systems and events, computer simulations are well suited to study this problem and have been used extensively to study different aspects of the translocation process. In this work, we present results from a system in which a polymer and a membrane containing a nanopore are placed in a medium containing obstacles. Using the Espresso Molecular Dynamics simulation package, simulations are performed in which the translocation events are driven by: i) an obstacle concentration gradient and ii) a varying amount of disorder. Results indicating the establishment of a preferential direction and assessing the impact of the system configuration on details such as the translocation time will be given.

1:51PM W20.00014 Role of RNA in the self-assembly of virus: A coarse-grained Brownian Dynamics study

Role of RNA in the self-assembly of virus: A coarse-grained Brownian Dynamics study

J.P. MAHALIK, MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Assembly of a single viral capsid (icosahedral T1 type) was studied in the absence and presence of RNA. A coarse-grained rigid body model was used to represent the capsomer units and a flexible polyelectrolyte model was used to represent RNA. Brownian Dynamics simulation was used to study the assembly process. The rate of assembly was found to be enhanced in the presence of RNA. The free energy contribution of the RNA in the self-assembly process was computed using weighted histogram analysis method.

2:03PM W20.00015 Probability of adsorption of peptide (CR3-1, S2) chains on clay minerals by coarse-grained Monte Carlo simulation

Probability of adsorption of peptide (CR3-1, S2) chains on clay minerals by coarse-grained Monte Carlo simulation

RAS B. PANDEY, University of Southern Mississippi, HENDRIK HEINZ, University of Akron, BARRY L. FARMER, SHARON JONES, LAWRENCE F. DRUMMY, RAJESH R. NAIK, Air Force Research Laboratory, WPAFB — A coarse-grained description is used to study the structure and dynamics of peptide chains (CR3-1, S2) in presence of a clay surface on a cubic lattice. A peptide chain is represented by the specific sequence of amino acids. Specificity of residues is captured via an interaction matrix based on the insight gained from the atomistic simulation, i.e., each residue interacts with surrounding residues, solvent, and the clay surface with a unique interaction potential. We use a standard LJ potential with its coefficient controlled by the interaction matrix. Simulations are performed with a number of peptide chains. Along with the global energy and dynamics of peptides, we keep track of mobility, energy (total and adsorption), and correlation with the local structure from the density profiles of each residue. Based on the analysis of local and global quantities, we are able to assess the probability of adsorption of peptides to clay surface in agreement with experiment. The probability of adsorption of S2 is found to be much higher than that of CR3-1 in which S2 is anchored by Lysine. The procedure is complementary to biopanning experiments since it allows screening a large number of peptides (more than 10E+5) on the surface to estimate their binding potential.
11:15AM W21.00001 Temperature Dependence of the Minority Carrier Lifetime in n− Epilayers of 4H-SiC, Paul Klein, Naval Research Laboratory, Amitesh Shrivastava, Tangali Sudarshan, University of South Carolina—Controlling the lifetime of minority carriers in n− epilayers of 4H-SiC is of great current interest, as short lifetimes lead to a high forward voltage drop in high-voltage, bipolar switching devices. As such devices operate at elevated temperatures, the temperature dependence of the carrier lifetime is of particular interest. For materials where the lifetime is controlled by trapping at deep defects (e.g., Z1/2Z2), increasing the temperature results in the thermal emission of trapped carriers, leading to an increase in the carrier lifetime. In this work the temperature dependence of the carrier lifetime, measured by time-resolved photoluminescence decay at low injection, has been studied in a range of epitaxial layers. In addition to the classic temperature dependence, some samples exhibit a lifetime that decreases rapidly with temperature in a thermally activated manner. This behavior is believed to result from the fact that the deep defect concentration is too low in these samples to limit the lifetime, and that other processes have become dominant.

11:27AM W21.00002 Issues with Deep Defect Spectra in Electron Irradiated 4H-SiC, F. Yan, R.P. Devaty, W.J. Choyke, Univ. of Pittsburgh, T. Kimoto, Kyoto Univ., T. Ohshima, Japan Atomic Energy Agency, G. Pensl, Univ. of Erlangen—Recently, Steeds et al. [1] discussed deep levels induced by high fluence electron irradiation in 4H-SiC. We have also observed the particular triplet assigned to di-carbon antisites using both ion implantation and electron irradiation. Here we specifically address data obtained by 170 keV electron irradiation at a fluence of 5×10^16 cm^-2. We shall discuss details of the no phonon lines of the triplet as well as two sets of vibrational modes well beyond the highest energy of the SiC lattice spectrum. Theory suggests that one should observe four no phonon lines and groups of four lines for each observed localized mode. Our high resolution spectra reveal differences in the LVM spectra with respect to those reported by Steeds et al. We obtain strong spectra at a fluence of 5×10^16 cm^-2 whereas Steeds et al. report that they do not see the triplet in the irradiated area using greater than 10^19 cm^-2, but do see it beyond the periphery of the TEM beam. We can explain this in terms of the transverse straggling of the electrons in his TEM beam. Finally, we report the reappearance of this triplet due to an anneal at 1100°C after it had already annealed out at 1400°C. [1] J. W. Steeds et al., Phys. Rev. B 77, 195203 (2008).

11:39AM W21.00003 Charge transfer kinetics of carbon vacancy defect in 4H-SiC, J. Dashdorj, M.E. Zvanut, J.G. Harrison, Department of Physics, University of Alabama at Birmingham—There has been much detailed work aimed at understanding carbon vacancy related defects and their complexes in SiC, but there are no reports of charge transfer kinetics between the carbon vacancy and other defect centers. In this study, optical cross sections of the positively charged carbon vacancy, V^+, in high purity semi-insulating 4H-SiC were measured by time-dependent photo-electron paramagnetic resonance, EPR. The measurements were performed by a X-band EPR spectroscopy at 80 K. Selected photon energies used in this study were between 0.8 and 3.13 eV. A single defect model considering only capture and emission of electrons from V^+ was shown to fit well the measured data. The photon energy-dependence of the cross sections exhibit threshold value of 1.6 eV and peak value of 2.15 eV for the capture, and threshold value of 1.9 eV and peak value of 2.45 eV for the emission processes, respectively. In this talk, we will discuss the above results in terms of charge transfer mechanisms including the effects of the electronic density of states and participation of phonons.

11:51AM W21.00004 EPR Study of SiC Defects Related to N2 and O2 Annealing, Sarah Thomas, Mary Ellen Zvanut, University of Alabama at Birmingham—SiC is a promising replacement for Si in future high power, high temperature electronic devices. It is well known that the Si/SiO2 interface in MOSFETS has electronically active defects, and recent work has shown the same is true for SiC. Our research focuses on identifying the cause and location of defects in thermally treated SiC substrates using EPR at 9.8 GHz. Samples underwent isochronal anneals from 400 to 1000 °C in pure nitrogen and oxygen ambients. Room temperature EPR spectra showed two defects, defect A and defect B, with line-widths of 4G and 10G, respectively. The temperature dependence was similar for the N2 and O2 anneals until 800 °C, when the concentration of defect A, which stayed constant in N2, decreased in O2. In both ambients defect B was eliminated, and it was determined that this defect was due to cutting. That the amount of defect A decreased during the O2 anneals, but not during the N2 suggests that oxidation, perhaps through etching, removes the signal. During the talk we will compare the results of oxidation and reactive ion etching studies, as these will give a better understanding of the location of defect A.

12:03PM W21.00005 Pulsed ENDOR at 240 GHz of nitrogen centers in 4H-SiC: towards a detailed description of the wavefunction, Johan Van Tol, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, Mary Ellen Zvanut, Department of Physics, University of Alabama at Birmingham, Birmingham, AL 35294-1170—SiC is a very suitable semiconductor material for high power and high temperature applications. The electronic properties of many different defects and dopants in various polytypes have been studied by electron paramagnetic resonance (EPR), including various common nitrogen substitutional defects. In particular, high frequency EPR has proven very powerful in separating the EPR signals of different sites, while the nuclear transitions of hyperfine coupled 29Si and 13C that are observed by electron nuclear double resonance (ENDOR) can be well separated. Here we report on new data on the hexagonal nitrogen center in 4H-SiC, for which the hyperfine interaction with the surrounding silicon and carbon shells was measured by pulsed ENDOR at 240 GHz. While these measurements give precise values for the electron spin density on the surrounding atoms, the assignment of these densities to particular atomic sites has proven challenging. The multiplicity and structure of the conduction band in this indirect semiconductor complicates the analysis. We will discuss the observed results and propose a tentative assignment on the basis of the Kohn-Luttinger theory. Supported by the NSF through grants DMR-0654118 and NSF DMR-0520481.

12:15PM W21.00006 X-ray photoelectron spectroscopy of Ni doped boron carbides, Nina Hong, Physics & Astronomy University of Nebraska-Lincoln, ma. Langell, Chemistry University of Nebraska-Lincoln, S. Adenwalla, Physics & Astronomy University of Nebraska-Lincoln—Ni acts as an n-type dopant for semiconducting boron carbide (BC). A series of samples with increased Ni doping were grown on Si substrates using plasma enhanced chemical vapor deposition (PECVD) and characterized using X measurements and X-ray photoelectron spectroscopy (XPS). Increased Ni doping leads to a linear increase in Ni concentration as evidenced by the intensity of the Ni 2p photoemission peak relative to that of the B 1s peak; concomitantly, the XPS curves indicate that the BC becomes increasingly n doped. B1s peak shapes shows B-C and B-B bonding structure, and the C1s peak shows B-C and C-C bond chains in all samples. The overall binding energies for B and C are consistent with the results from sputter deposited stoichiometric B,C [1]; in these PECVD grown samples, however, the graphite peak commonly seen in the sputter deposited BC is absent. [1] I Jimenez, L. J. Terminello, et al. J. Elect. Spec. Relat. Phenom., 101-103, 611-615 (1999).

3Supported by NSF-0725881 and NASA NNG05GM89G.
First-principles study of Oxygen vacancies in Mg,Zn\textsubscript{x}O alloys, ADISAK BOOCHUN, WALTER LAMBERT. Case Western Reserve University — A first-principles study of oxygen vacancies in Mg,Zn\textsubscript{x}O alloys has been carried out within the LDA+U + E\textsubscript{dd} FP-LMTO approach. Different types of oxygen vacancies are distinguished by their number of Mg and Zn nearest neighbors. We find that the energy of formation is lowest for oxygen vacancies surrounded by four Zn nearest neighbors. Because of the Boltzmann factor this implies that the probability of finding oxygen vacancies with one or more Mg as nearest neighbors is strongly suppressed. Unlike in pure ZnO and MgO, we do not find negative U behavior but this may in part be because of the small size of the supercell. The 2+/+ and +/0 transitions level gradually move to higher energy as the number of nearest neighbor Mg atoms increases. Defect levels in rocksalt MgO are also presented.

Cation dopant distributions in m-doped ZnO nanostructures and thin films: experiment and Monte Carlo simulations, T.C. DROUBAY, PACIFIC NORTHWEST NATIONAL LAB, D.J. KEAVNEY, S.M. HEALD, ARGON NATIONAL LAB, T.T. KASPAR, B.P. KASPAR, C.M. WANG, PACIFIC NORTHWEST NATIONAL LAB, C.A. JOHNSON, K.M. WHITAKER, D.R. GEMALINI, CHEMISTRY, UNIV. OF WASHINGTON, S.A. CHAMBERS, PACIFIC NORTHWEST NATIONAL LAB — Anion or cation doping at relatively high concentrations of several atomic percent is frequently suggested to realize synthetic materials with qualitatively new functionality. While the statistical probability of obtaining singles, dimers, and trimers has been determined for bulk lattices, these distributions are significantly altered in nanostructures and thin films due to the presence of under-coordinated surface sites. The dopant distributions in nanostructures and thin films of doped wurtzite ZnO have been determined from Monte Carlo simulations. Using empirical expressions derived from the MC simulations that accurately predict dopant bonding configurations as a function of surface-volume ratio and concentration, experimental results for epitaxial films of Mn-doped ZnO will be discussed. X-ray absorption and x-ray magnetic circular dichroism revealed that Mn(II) substituted for Zn in the Mn:ZnO films, which were deposited by PLD using targets created from Mn:ZnO nanoparticles. However, while substitutional, the Mn distribution is not stochastic but rather tends to segregate, yielding higher local concentrations than anticipated.

Weak localization effects in Al-doped ZnO films, PRIYA.V CHINTA*, Q.Y. CHEN*, O. LOZANO*, P.V. WADEKAR*, W.K. CHU, PACIFIC NORTHWEST NATIONAL LAB, D.J. KEAVNEY, S.M. HEALD, ARGON NATIONAL LAB, T.T. KASPAR, B.P. KASPAR, C.M. WANG, PACIFIC NORTHWEST NATIONAL LAB, C.A. JOHNSON, K.M. WHITAKER, D.R. GEMALINI, CHEMISTRY, UNIV. OF WASHINGTON, S.A. CHAMBERS, PACIFIC NORTHWEST NATIONAL LAB — Metal-semiconductor transitions (MST) at low temperatures were studied for Zn\textsubscript{1−x}Al\textsubscript{x}O thin films deposited by simultaneous RF magnetron sputtering of ZnO and Al onto (11-20)-oriented Al\textsubscript{2}O\textsubscript{3} substrates. The MST occurs at 100K, 102K and 260K for x = 2%, 3% and 10% of Al-doping, respectively. The samples display negative magnetoresistance at low temperatures with zero-field electrical resistivity as low as 3.3 × 10\textsuperscript{-4} Ω cm for x = 3%. The charge scattering mechanisms below the MST will be discussed in light of weak localization and coulomb interactions due to disorder in the system. *Also with Dept of Physics, NSYSU, Taiwan.

First-Principles Theoretical Analysis of Dopant Adsorption and Diffusion on Surfaces of II-VI Compound Semiconductor Nanocrystals, TEJINDER SINGH, J. T. MOUNTZIARIS, DIMITRIOS MAROUDAS, UNIVERSITY OF MASSACHUSETTS, AMHERST — We present a first-principles theoretical analysis of dopant adsorption, and diffusion on facets of II-VI semiconductor nanocrystal surfaces and discuss its implications for dopant incorporation into growing nanocrystals. We focus on ZnSe nanocrystals with diameters d ∼ 5 nm that have polyhedral shapes with well-defined facets. Using density functional theory calculations, we find that the binding energy for Mn adsorption onto various sites of the ZnSe(001)-(2×1) surface increases with increasing dopant surface concentration. This low binding energy at low dopant concentration provides an explanation for dopant diffusion during nanocrystal growth. In addition, we have analyzed several dopant migration pathways for Mn diffusion on the ZnSe(001)-(2×1) surface and calculated the corresponding activation barriers as a function of dopant surface concentration. We find that Mn atoms can migrate fast along the Se dimer rows. However, Mn migration to a trough site is governed by a high-barrier process that may lead to dopant incorporation into the ZnSe nanocrystal.

Effect of Oxygen Vacancies in In\textsubscript{2}O\textsubscript{3}, KALUM PALANDAGE, DEPARTMENT OF PHYSICS, UNIVERSITY OF CONNECTICUT, ADILGER KUSSOW, DEPARTMENT OF PHYSICS, UNIVERSITY OF MASSACHUSETTS LOWELL, ALKIM AKYURTLU, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, UNIVERSITY OF MASSACHUSETTS LOWELL, GAYANATH FERNANDO, DEPARTMENT OF PHYSICS, UNIVERSITY OF CONNECTICUT — In order to assess the effect of oxygen vacancies on its electronic structure, we have calculated the band structure of In\textsubscript{2}O\textsubscript{3} (in the I\textsubscript{a}3 structure) with and without oxygen vacancies using density functional theory within the local density approximation. A 4 × 4 × 1 Monkhorst-Pack grid of k-points was used to sample the Brillouin zone while permitting full structural relaxation and self-consistency. A noticeable change that is observed is in the nature of the direct band gap of In\textsubscript{2}O\textsubscript{3} at the zone center, which becomes indirect with the addition of a single oxygen vacancy to an ideal 40-atom unit cell. There is also a clear tendency toward metallic behavior with the inclusion of a single oxygen vacancy, which appears to be independent of the location of the vacancy. In addition, spin-polarized calculations reveal negligible magnetic moments due to the introduction of these vacancies. The threshold vacancy concentration necessary for metallic behavior, our results from a symmetry analysis of the relevant valence and conduction band states, which are crucial for optical transitions, as well as effects due to Cr-doping will be presented.

Transport properties of transparent conducting oxide thin film, Nb:In\textsubscript{2}O\textsubscript{3}, O. LOZANO*, Q.Y. CHEN*, P.V. WADEKAR*, L.H. CHU, W.J. WIESUNDERA, WEI-KAN CHU, DEPARTMENT OF PHYSICS AND CENTER FOR NONSCIENCE AND NANOTECHNOLOGY, NATIONAL SUN YAT-SEN UNIVERSITY, KAOHSIUNG, TAIWAN, REPUBLIC OF CHINA, S.W. YEH, N.J. HO, DEPARTMENT OF MATERIALS AND OPTOELECTRONIC SCIENCES AND CENTER FOR NANOSCIENCE AND NANOTECHNOLOGY, NATIONAL SUN YAT-SEN UNIVERSITY, KAOHSIUNG, TAIWAN — Thin films of Nb-doped In\textsubscript{2}O\textsubscript{3} were deposited on YSZ(001) by magnetron co-sputtering. The well-oriented thin films were studied as a function of Nb concentration by optical absorption spectroscopy and magneto-optical transition measurement. The optical transparency in the visible and infrared spectral ranges is 97−99% while the electrical resistivity is about 0.4 mΩ·cm. The variation of these properties with respect to doping will be discussed in the context of scattering and optical transition mechanisms. *Also with Department of Physics and Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China.

A First-Principle Density-Functional Theory of BxGa\textsubscript{1−x}BiyAs\textsubscript{1−y} Quaternary Alloys, ZUOZI CHEN, U.C. Berkeley and LBNL, LEI LIU, U.C. Berkeley, LBNL, and Nanyang Technical University, PETER Y. YU, U.C. Berkeley and LBNL, ZHI XUN MA, LBNL, S.S. MAO, U.C. Berkeley and LBNL, ZHILIAN WANG, LBNL, ZHUOZI CHEN, U.C. Berkeley and LBNL, LEI LIU, U.C. Berkeley, LBNL, and Nanyang Technical University, PETER Y. YU, U.C. Berkeley and LBNL, ZHI XUN MA, LBNL, S.S. MAO, U.C. Berkeley and LBNL — Both B and Bi are isovalent impurities in GaAs when they substitute for Ga and As, respectively, at low concentrations. At higher concentrations they can form alloys with GaAs. They have opposite effects on the host GaAs crystal in terms of the lattice constant and band gap. B is smaller than Ga and will increase the band gap of GaAs in addition to converting it from a direct band gap semiconductor into an indirect one. On the other hand, Bi is larger than As and will decrease the band gap of GaAs, turning it into a semi-metal at high concentration. In principle, by incorporating B and Bi into GaAs in appropriate concentration one can tune the band gap of the alloy over a large range of values from the far infra-red to the near uv. We have performed a first-principle density-functional calculation of the total energy, lattice parameters and the band gap of the cubic BxGa\textsubscript{1−x}BiyAs\textsubscript{1−y} alloy system. A generalized quasi-chemical approach is adopted to handle the disorder effects induced by alloying. The dependence of band gap energy surface Eg(x,y) of the quaternary alloy was also obtained. The restriction of a single oxygen vacancy, which appears to be independent of the location of the vacancy. In addition, spin-polarized calculations reveal negligible magnetic moments due to the introduction of these vacancies. The threshold vacancy concentration necessary for metallic behavior, our results from a symmetry analysis of the relevant valence and conduction band states, which are crucial for optical transitions, as well as effects due to Cr-doping will be presented.

Research supported by the U.S. Department of Energy, NNSA/NA-22, under Contract No. DE-AC02-05CH11231.


into regions more or less rich in the magnetic component, and that can be controlled by the growth parameters and co-doping with shallow donors and acceptors into the nitride matrix in a way giving rise either to a diluted random alloy or to ferromagnetic nanocrystals that aggregate by precipitation or by spinodal decomposition of a renormalization of extended states occurring if the impurities perturb strongly the crystal potential. We then show that the Fe ions are incorporated in the

formation on the Fe distribution at the nanoscale. In this talk, we first discuss our quantitative study of the exchange coupling between the spins S = 5/2 localized exhibiting spintronic functionalities has resulted in the discovery of a number of magnetically doped or nominally undoped wide-band gap semiconductors and

ductors. The case of (Ga,Fe)N

11:51AM W21.00004 Diffusion of point defects in CdTe

JOHN JAFFE, CHARLES HENAGER, Pacific Northwest National Lab — We have investigated the mobility of isolated native point defects in CdTe by first-principles calculations. Cd vacancies and interstitials, Te interstitials and Te-on-Cd antisites were considered. Diffusion barriers were found by the NEB (nudged- elastic-band) technique within the PAW-LDA method as implemented in the VASP code. Diffusion constants are estimated, and some implications for the growth of radiation detector material are suggested, especially in regard to the formation of Te precipitates. Comparisons to experimental and earlier theoretical studies are also provided.

11:15AM W22.00001 Nitrogen defects and ferromagnetism in Cr-doped AlN

BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — It is believed that N defects play important roles in achieving high-temperature ferromagnetism in Cr-doped AlN. We use state-of-the-arts DFT method to investigate N defects and their effects on ferromagnetism of (Al,Cr)N with N vacancies \( V_N \). Our total-energy calculations show that the nearest Cr-Cr pair with the two spins in parallel is the most favorable and the nearest Cr-\( V_N \) pair makes a stable complex. Our formation energies indicate that \( V_N \) regions can be formed spontaneously under N-poor condition, or Cr-doped regions can be formed under N-rich condition. Hence real samples should be inhomogeneous. Both of the single Cr and \( V_N \) create filled electronic states in the semiconductor gap of AlN. N vacancies enhance the ferromagnetism by enlarging Cr moment, but reduce the ferromagnetic exchange constants between the spins in the nearest Cr-pair. These calculated results are in agreement with experimental observations and facts. Phys. Rev. B 78, 195206 (2008).

11:27AM W22.00002 Optical and magnetic properties of Tm-doped doped AlGaN alloys

N. NEPAL, S.M. BEDAIR, J.M. ZAVADA, Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695 USA, N.A. EL-MASRY, Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695 USA, D.S. LEE, A.J. STECKL, Electrical and Computer Engineering, Texas Tech University, Lubbock, Texas 79409, USA — Trivalent RE-ions in AlGaN alloys have been shown to emit narrow intra-4f transitions over the entire infra red to ultraviolet (UV) spectral range. Also, unpaired 4f-electrons of RE ions can align along an easy axis giving magnetic properties to these RE-doped semiconductors. Thulium is one of the RE elements which has an easy magnetic axis, and we study its optical and magnetic properties of Tm-doped Al\(_{x}\)Ga\(_{1-x}\)N \((0 \leq x \leq 1)\) alloy grown by solid-source molecular beam epitaxy. We present optical and magnetic properties of Tm-doped Al\(_{x}\)Ga\(_{1-x}\)N \((0 \leq x \leq 1)\) alloys.

11:39AM W22.00003 The Failure of LDA and GGA to describe Relative Stability, Electronic Structure and Magnetism of MnN and (Ga,Mn)N Alloys

JENNIFER CHAN, ZHE ZHOU, LIU HANNES RAEBIGER, STEPHAN LANY, ALEX ZUNGER, NREL, Golden, CO 80401 — Pure MnN and (Ga,Mn)N alloys are studied using \( \textit{ab initio} \) generalised gradient approximation +U (GGA+U) or hybrid-exchange density functional (B3LYP) methods which predict dramatically different electronic structure, magnetic behavior and relative stabilities compared to local-density calculations. A unique structural anomaly of MnN, in which local-density calculations fail to predict the experimentally observed rocksalt as the ground state, is resolved with GGA+U and B3LYP. The phase-separation of zinc-blende (Ga,Mn)N alloys is examined using a mixed-basis cluster expansion based on the corrected GGA total energies. The predicted asymmetric spinodal phase diagram indicates that (Ga,Mn)N precipitates contain \%50 Mn at typical growth temperatures. Thus, 100% pure MnN, that suppresses the Curie temperature, will not be formed. The Curie temperature for the \( x_{\textit{fit}}=50\% \) phase is estimated to be \( T_C=\sim 300 \text{ K} \) indicating that high \( T_C \) ferromagnetism in zinc-blende (Ga,Mn)N alloys is due to precipitates.


Session W22 GMAG DMP FIAP: Focus Session: Dilute Magnetic Nitride Semiconductors

Thursday, March 19, 2009 11:15AM - 1:51PM

11:51PM W21.00014 Diffusion of point defects in CdTe

JOHN JAFFE, CHARLES HENAGER, Pacific Northwest National Lab — We have investigated the mobility of isolated native point defects in CdTe by first-principles calculations. Cd vacancies and interstitials, Te interstitials and Te-on-Cd antisites were considered. Diffusion barriers were found by the NEB (nudged- elastic-band) technique within the PAW-LDA method as implemented in the VASP code. Diffusion constants are estimated, and some implications for the growth of radiation detector material are suggested, especially in regard to the formation of Te precipitates. Comparisons to experimental and earlier theoretical studies are also provided.

2:03PM W21.00015 Engineering Oxygen Vacancy Distribution by Exteranal Strain

DA-JUN SHU, SHU-TING GE, MU WANG, NAI-BEN MING, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China — The most common defects on surfaces are transition metal oxides are oxygen vacancies, which play critical roles in applications such as heterogeneous catalysis, photoelectrolysis, biocompatibility, etc. If the nature and distribution of the oxygen vacancies can be controlled, the surface properties will then be modified for different applications. For this purpose, one needs to understand both the influence of oxygen vacancies on the surface properties and the responses of oxygen vacancies to different external fields. We have conducted comprehensive first principles calculations on the surface energy of strained rutile TiO2(110) with oxygen vacancies. The formation energy of each type of oxygen vacancy is calculated as a function of external strain. We find that the type of the most easily formed oxygen vacancy can be tuned by the strain and therefore suggest that the distribution of oxygen vacancies can be engineered by external strain, which helps to improve the applications of TiO2 surface where oxygen vacancies play important roles. The dependence of surface elastic properties on the type of oxygen vacancy is found to be responsible for the interplay between external strain and oxygen vacancies.

2:39PM W21.00016 Origin and control of ferromagnetism in magnetically doped semiconductors. The case of (Ga,Fe)N

ALBERTA BONANNI, Johannes Kepler University - Linz — The comprehensive search for materials exhibiting spintronic functionalities has resulted in the discovery of a number of magnetically doped or nominally undoped wide-band gap semiconductors and oxides showing ferromagnetic features persisting up to high temperatures. In order to shed light on the origin of the high-TC ferromagnetism in these materials systems, we have undertaken studies of MOVPE-grown (Ga,Fe)N, either undoped or co-doped with Si or Mg, combining the magnetic (SQUID and EPR), magnetoeoptical, and XANES investigation with a thorough structural and chemical characterization (SIMS, TEM, EDS, synchrotron XRD), that provides information on the Fe distribution at the nanoscale. In this talk, we first discuss our quantitative study of the exchange coupling between the spins \( s = 5/2 \) localized on the Fe ions and of the effective mass electrons. Our results point to an anomalous p-d exchange splitting of the valence band [1], that we explain in terms of a renormalization of extended states occurring if the impurities perturb strongly the crystal potential. We then show that the Fe ions are incorporated in the nitride matrix in a way giving rise either to a diluted random alloy or to ferromagnetic nanocrystals that aggregate by precipitation or by spinodal decomposition into regions more or less rich in the magnetic component, and that can be controlled by the growth parameters and co-doping with shallow donors and acceptors [2].


1. Supported by DOE DOE National Nuclear Security Administration NA-22.

2. Funded by the DOE-SC-BES-MSED and the DARPA-PROM program under NREL contract DE-AC36-08GO28308.
12:27PM W22.00005 Magnetic, structural and optical properties of Mn-based and Cr-based diluted magnetic semiconductors and alloys. A. ALSAAD, Jordan University of Science and Technology — We have implemented supercell approach by using local spin density functional theory for Mn-doped GaN, Mn-doped ScN and the linear muffin-tin orbital method to predict the structural and magnetic properties of these novel diluted magnetic semiconductors and their Ga$_{1-x}$Mn$_x$N and Sc$_{1-x}$Mn$_x$N alloys. The global energy minimum of MnN is obtained for zinc-blende structure. If the compound is compressed by 6 % the energy minimum corresponds to the NaCl structure in disagreement with the experimentally observed a slightly tetragonally distorted rocksalt structure, known as α phase. The rocksalt structure of CrN at about 8 % lattice expansion becomes stable in the ferromagnetic (FM) state and has a global minimum energy at a lattice constant of 3.9 Å. We have observed an isostructural phase transition for Sc$_{1-x}$Mn$_x$N alloys from zince-blende phase to hexagonal phase that occurs at a hydrostatic pressure of 17.5 GPa. Moreover, the structural and optical properties of single crystal CrN/ScN superlattices and C$_{1-y}$S$_y$N alloys are studied in details. We report an isostructural phase transition from wurzite (w-CrN) to hexagonal (h-ScN) at a hydrostatic pressure of 21 GPa. We have also used first-principles methods to study the electronic, optical and magnetic properties of MnN and MnAs compounds in the hypothetical cubic zinc-blende phase, a phase in which the two MnN and MnAs binaries have the same local environment as that they have in GaMnN and GaMnAs alloys. We show that MnN exhibits antiferromagnetic (AFM) ground state and MnAs adopts ferromagnetic (FM) ground state.

12:39PM W22.00006 Role of the Localized Defect States in the Unconventional Magnetism of GaN and ZnO. PRATIBHA DEV, PEIHONG ZHANG, Physics Department, University at Buffalo, Buffalo, NY 14260 — The cation defects -vacancies and the appropriate substitutionals - introduce localized defect states chiefly centered around the four surrounding anions in GaN and ZnO. This defect-induced magnetism in these otherwise nonmagnetic semiconductors is studied using ab-initio methods. The defects investigated include the cation vacancy, substitutional acceptors, and acceptor-like defect complexes. The defect states show two opposing attributes -one on one hand, they are strongly localized on the anions surrounding the defect site, leading to local magnetic moment formation, while on the other hand, the extended tails of their wavefunctions lead to the long-ranged exchange interaction between the local moments.

12:51PM W22.00007 Defect induced ferromagnetism in Gd doped GaN. CHANDRIMA MITRA, WALTER LAMBRECHT, Case Western Reserve University — We review various suggested mechanisms for the ferromagnetism in Gd-doped GaN using local spin density approximation supercell calculations. The spin splitting of the conduction band induced by the Gd s − f coupling is found to decrease linearly with Gd concentration and hence colossal magnetic moments cannot be explained by explaining this spin-split band with ionized donor electrons. Furthermore, we find the Gd-Gd interactions to be antiferromagnetic except in p-type material. Although, Ga vacancies can induce long range interactions and up to three Bohr magneton moments per vacancy in the neutral charge state, we note that these defects only are favorable to form in n-type materials and then should predominantly occur in a 3− charge state which has no magnetic moment. N-interstitials are likely to form in conjunction with N vacancies for mid gap Fermi levels consistent with the semi-insulating nature of the samples and have a magnetic moment for the corresponding charge state. We find that Gd in the presence of N interstitials alone prefer antiferromagnetic coupling but in the present of both N-interstitials and N vacancies prefer ferromagnetic coupling. We find that oxygen tends to segregate toward an interstitial site near the Gd and in that case can induce a strong ferromagnetic coupling between Gd.

1:03PM W22.00008 Ferromagnetism in GdN: an antiferromagnet in disguise. WALTER R. L. LAMBRECHT, CHANDRIMA MITRA, Case Western Reserve University — We analyze the exchange interactions in GdN and Gd pnictides GdX with X=P,As,Sb,Bi to the long-ranged exchange interaction between the local moments.

1:15PM W22.00009 Ferromagnetism and Photoluminescence in Rare-Earth doped GaN via Diffusion. M. OLIVER LUEN, N. NEPAL, S.M. BEDAIR, J.M. ZAVADA, Electrical and Computer Engineering, North Carolina State University, Raleigh, NC 27695 USA, EL EI BROWN, U. HOMMERICH, Department of Physics, Hampton University, Hampton, VA 23686 USA, P. FRAJTAG, N.A. EL-MASRY, Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695 USA — Rare-earth doped GaN is attracting attention both as a diluted magnetic semiconductor (DMS) material and for optical devices useful in communications and multi-color semiconductor display technology. GaN’s large band gap (3.4 eV) gives rise to optical transparency over a wide spectral range, from the infrared (IR) to the ultraviolet. These properties make it an optimum host for the various emissions that are possible from rare-earth (RE) ions. Recently, rare-earth doped GaN also has demonstrated above room temperature ferromagnetism. In this study, we report the diffusion of RE (Nd, Sm, Gd and Er) into undoped, Mg-doped and Si-doped GaN templates. Room temperature optical and ferromagnetic properties were studied using photoluminescence (PL) and alternating gradient magnetometer, respectively. Ferromagnetic properties show a preference for undoped and n-type GaN. PL spectra exhibit RE ion inner shell transitions in the visible and infrared regions. The mechanisms for above room temperature ferromagnetism and emission intensity related to the RE concentration, is discussed.

1:27PM W22.00010 Dilute Magnetic and Electronic Properties of Mn$_{0.25}$Sc$_{0.75}$N/ScN(001)/MgO(001) Films Grown by Molecular Beam Epitaxy. COSTEL CONSTANTIN, Seton Hall University, KANGKANG WANG, ABHIJIT CHINCHORE, ARTHUR SMITH, Ohio University, HAN-JONG CHIA, JOHN MARKERT, University of Texas at Austin — In this study, we report the magnetic and electronic properties of Mn$_n$Sc$_{1-n}$N films grown by molecular beam epitaxy. Recently, theoretical calculations predicted a Curie temperature above 350 K for ScN films with up to 20% Mn impurity concentrations[1]. The magnetic hysteresis data suggests ferromagnetic behavior for Mn$_{0.03}$Sc$_{0.97}$N and Mn$_{0.15}$Sc$_{0.85}$N films with Curie temperatures of 383 K and 361 K, respectively. Furthermore, the measured electron concentrations for the Mn$_{0.03}$Sc$_{0.97}$N and Mn$_{0.15}$Sc$_{0.85}$N films are 6.51×10$^{19}$ cm$^{-3}$ and 6.17×10$^{19}$ cm$^{-3}$, respectively. These measured carrier concentration agree well with the prediction of Herwadkar et al. that ferromagnetism above room temperature in Mn$_{1-n}$Sc$_n$N should be possible by keeping the electron concentration below 10$^{20}$ cm$^{-3}$. This work is supported by: Seton Hall: University Research Council; Ohio University: DOE-BES Grant No. DE-FG02-06ER46317 and NSF Grant No. 0730257; and UT Austin: NSF Grant Nos. DMR-0605828 and DGE-0549417, Welch Foundation Grant No. F-1191. [1] A. Herwadkar (et al.), Phys. Rev. B 77, 134433 (2008).
11:15AM W23.00001 Pressure-induced structural transitions in the potential hydrogen storage compound NH$_3$BH$_3$ \(^{1}\). RAVHI KUMAR, HIPSEC, University of Nevada Las Vegas, JIANZHONG ZHANG, MONIKA HARTL, ZHUJUN LIN, SVEN VOGEL, LUKE DAEMEN, LANSCOE, ANDREW CORNELIUS, MALCOLM NICOI, HIPSEC, University of Nevada Las Vegas, YUSHEN ZHAO, LANSCOE — Ammonia borane has received much attention in recent years as it is reported to have up to 19.6 wt % of hydrogen \(^{1-2}\). Hydrogen is released in a three step process when heated above 100°C. To understand the structural stability of this compound under compression, we have performed high pressure angle dispersive x-ray diffraction experiments up to 27 GPa using synchrotron x-rays at HPCAT, Advanced Photon Source. Two successive pressure induced structural phase transitions were observed. The ambient tetragonal structure transforms to an orthorhombic structure around 1.2 GPa and then to another high pressure phase above 8 GPa. Complementary neutron diffraction experiments performed up to 5 GPa at LANSCOE are in good agreement with the x-ray results. The structural details of the high pressure phases will be presented.

\(^{1}\)This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy.
12:27PM W23.00007 Quasi-isentropic Compression Waves Generated by Shock Waves into Sapphire

W. J. NELIS, Harvard University, G. I. KANELO, S. V. RAZORENOV, A. S. SAVINYKH, Institute for High Temperatures, A. M. RAJENDRAN, U. Mississippi — For sixty years it has tacitly been assumed that a shock wave incident on a material will propagate as a shock wave in that material. Between 15 and 80 GPa a shock wave cannot propagate in sapphire, the first material demonstrated not to have a Hugoniot. Wave profiles of sapphire crystals with three orientations and two thicknesses were measured at incident shock stresses of 14, 24 and 87 GPa. 14 GPa generates elastic shocks that are overdriven at ~90 GPa. Elastic-precursor decay occurs at 24 and 87 GPa. At 24 GPa all three orientations have plastic-compression waves with rise times of 200-300 ns. Long rise times are probably caused by strong bonds that break heterogeneously and statistically over a relatively long time interval. This slow damage-induced increase in pressure causes quasi-isentropic compression. Since the Hugoniot and isotherm of sapphire are essentially coincident up to 340 GPa, dissipative energy probably goes primarily into entropy of disordering the crystal rather than temperature.

1Work supported by USARO Grants W911NF0610517 and CRDF 1668.

12:39PM W23.00008 Micron scale simulations of a Kelvin-Helmholtz instability: a direct comparison between molecular dynamics and Navier-Stokes hydrodynamics.

VICTOR PARDO, DANIEL BALDOMIR, Applied Physics Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, ARTURO MANUEL BANOBRE, Physical Chemistry Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, ALBERTO PINEIRO, MOSEY, University of Kingston, YANG SONG, PETER NORTON, MARTIN MUESER, University of Western Ontario — In this study, we present X-ray diffraction data on zinc- and calcium phosphates. The experiments reveal that low-coordinated zinc phosphates are good anti-wear agents.

12:51PM W23.00009 Transition of deformation modes in Shocked Tantalum

LUKE HSIUING, Lawrence Livermore National Laboratory — Shock-induced twinning and α (bcc) → ω (hexagonal) phase transition in tantalum, which exhibits no clear solid-state phase transformation under hydrostatic pressure conditions, have been investigated. Since the domains of deformation twin and ω phase were frequently observed in experiments conducted at high pressure and small strain, we simulate shock wave propagation through dislocation-cell structures. It is suggested that the shock-induced shear transformations (twinning and phase transformation) occur as alternative deformation modes to accommodate insufficient dislocation flow resulting from the exhaustion of dislocation multiplication when dynamic recovery processes for dislocation annihilation and cell formation become largely suppressed under dynamic pressure conditions. A physical mechanism based upon the overlapping of closely spaced dislocation loops nucleated from a jogged screw dislocation is proposed to rationalize the shock-induced shear transformations. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

1:03PM W23.00010 Hydrogen at Extreme Conditions

SUBRAMANIAN NATARAJAN, ALEXANDER CONCHAROV, SOMAYAZULU MADDURY, RUSSELL HEMLEY, Geophysical Laboratory, Carnegie Institution of Washington, Washington DC 20015 — Vast regions of the P-T phase diagram of H₂, especially in the high P-T region, remain to be explored for melting behavior and exotic phenomena related to dissociation of the H₂ molecule, metallicity and superconductivity. In recent years, few experiments employing either laser-heating or resistive heating techniques in conjunction in situ spectroscopic experiments using Diamond Anvil Cells (DAC) have been reported attempting to address some of these. A key problem that faces experimenters is to confine the hot and reactive H₂ in the small DAC sample chamber at high pressures long enough to make meaningful measurements of physical properties. Recently, we have made considerable progress in confining hot and dense hydrogen while not compromising on the ability to make spectroscopic measurements using a complex sample assembly. With this, it has been possible to perform in situ Raman spectroscopy on H₂ and D₂ while simultaneously doing double-sided laser heating at P-T conditions of more than 1Mbar and 1500K. Typically, we are now able to perform laser heating and in situ Raman spectroscopy over several heating/cooling cycles without loss of H₂ in the Mbar range. Results of these experiments will be presented; along with details of the methodology we adopted to successfully confine hot and dense hydrogen.

1:15PM W23.00011 An accurate high pressure scale from quantum Monte Carlo

KENNETH ESLER, R.E. COHEN, Geophysical Laboratory, Carnegie Institution, BURKHARD MILITZER, Dept. of Astronomy, UC Berkeley, JEONGNIM KIM, University of Illinois at Urbana-Champaign, NCSA — We have developed a fundamental high-temperature and high-pressure scale based on cubic boron nitride (cBN) using a combination of Quantum Monte Carlo (QMC) for the static contribution along with density functional perturbation theory (DFPT) for the thermal pressure. The anharmonic Raman frequency was determined as a function of pressure by solving the Schroedinger equation for the vibrational well determined using QMC combination of Quantum Monte Carlo (QMC) for the static contribution along with density functional perturbation theory (DFPT) for the thermal pressure. The QMCPACK code. We include a novel correction based on all-electron wave functions to eliminate pseudopotential error.

1:27PM W23.00012 Softening of ultra-incompressible CrN at high pressure

FRANCISCO RIVADULLA, MANUEL BANOBRE, Physical Chemistry Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, ALBERTO PINEIRO, TICTOR PARDO, DAVIEL BALDOMIR, Applied Physics Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, ARTURO LOPEZ-QUINTELA, Physical Chemistry Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain, JOSE RIVAS, Applied Physics Department, University of Santiago de Compostela, 15782 Santiago de Compostela, Spain — We report a dramatic softening of CrN above 1.5 GPa, (the bulk modulus decreasing from K=4.0 GPa to 2.4 GPa) associated to a structural transition. From the structural and magnetic data under pressure, and ab-initio calculations we suggest that this effect is purely electronic, driven by the proximity of the ionic Cr-Cr bond to itinerant electron limit. Our results help to understand fundamental aspects of the chemical bond that gives superhard materials their superior mechanical properties, and could be useful to preserve the mechanical properties of CrN.

1:39PM W23.00013 Correlating cation coordination, stiffness, phase transition pressures, and smart materials behavior in metal phosphates

DMITRY SHAKHROVOSTOV, University of Western Ontario, NICHOLAS MOSEY, University of Kingston, YANG SONG, PETER NORTON, MARTIN MUESER, University of Western Ontario — In this study, we present X-ray diffraction data on zinc- and calcium phosphates. The experiments reveal that low-coordinated zinc phosphates are relatively soft at ambient conditions but stiffen dramatically with increasing pressure, p, exhibiting smart materials behavior, while high-coordinated zinc and calcium phosphates have higher initial bulk moduli and stiffen considerably less rapidly with increasing p. All systems amorphize when their bulk modulus reaches a value near 210 ± 40 GPa, where the precise value depends on chemical details, indicating that phosphate networks become unstable when their bulk modulus reaches that value. Our ab-initio simulations of zinc-α-phosphate support the idea that the elastic properties are controlled by the motion of rigid phosphate units, which becomes more hindered under densification, with or without increasing cation coordination. It is discussed how these results may explain why low-coordinated zinc phosphates are good anti-wear agents.
1:51PM W23.00014 Novel Numerical Computations for the Equation of State of Hard Particle Systems from Gaseous to Extreme High Densities, UDUZEI EDGAL, Old Dominion University — A special form of the “Reduced Monte Carlo Scheme” (RMCS) used for numerical computation of the EOS of the hard particle system (2D and 3D cases) will be discussed. A major advantage of the numerical scheme is that it does not lead to difficulties with meta-stable states as do traditional MC methods. In particular, RMCS calculations (in the special form) provide results from the lowest (fluid phase) to the highest (solid phase) densities which show a first order phase transition in the hard particle system.

2:03PM W23.00015 X-ray diffraction of electrodeposited nanocrystalline Ni under high-pressure, CHRISTIAN GRANT, Livermore National Laboratory, JONATHAN CROWHURST, TOM ARSENLIS, Lawrence Livermore National Laboratory, EDUARDO BRINGA, Instituto de Ciencias Basicas Universidad Nacional de Cuyo, MORRIS WANG, JAMES HAWRELIK, PETER PAUZAUSKIE, Lawrence Livermore National Laboratory, SIMON CLARK, Advanced Light Source, Lawrence Berkeley National Laboratory — We studied the compressibility of monolithic fully-dense electrodeposited nanocrystalline Ni (29 nm grain size) under both quasi-hydrostatic and non-hydrostatic conditions up to a nominal pressure of 50 GPa using angle-dispersive x-ray diffraction. We obtained an equation of state consistently and unambiguously from each measured reflection. The apparent bulk modulus measured under non-hydrostatic conditions is larger than that of the corresponding coarse grained-material under either type of compression, but is nearly the same when measured under quasi-hydrostatic conditions. Our results suggest that the strength, but not the bulk modulus, of 29 nm crystalline Ni is enhanced relative to its coarse-grained counterparts.


11:15AM W24.00001 Quantum Monte Carlo Studies of Interaction-Induced Localization in Quantum Dots and Wires, A. DEVIRM GÜÇÜL, Institute for Microstructural Sciences NRC, Ottawa and Duke University — We investigate interaction-induced localization of electrons in both quantum dots and inhomogeneous quantum wires using variational and diffusion quantum Monte Carlo methods. Quantum dots and wires are highly tunable systems that enable the study of the physics of strongly correlated electrons. With decreasing electronic interaction-induced localization of electrons in both quantum dots and inhomogeneous quantum wires using variational and diffusion quantum Monte Carlo methods. Quantum dots and wires are highly tunable systems that enable the study of the physics of strongly correlated electrons. With decreasing electronic interactions, electrons become stronger and electrons are expected to localize at their classical positions, as in Wigner crystallization in an infinite 2D system. (1) Dots: We show that the addition energy shows a clear progression from features associated with shell structure to those caused by commensurability of a Wigner density, interactions become stronger and electrons are expected to localize at their classical positions, as in Wigner crystallization in an infinite 2D system. (1) Wires: We study an inhomogeneous quasi-one-dimensional system—a wire with two regions, one at low density and the other high. We find that strong localization occurs in the low density quantum point contact region as the gate potential is increased. The nature of the transition from high to low density depends on the density gradient—if it is steep, a barrier develops between the two regions, causing Coulomb blockade effects. We find no evidence for ferromagnetic spin polarization for the range of parameters studied. The picture emerging here is in good agreement with the experimental measurements of tunneling between two wires. Collaborators: C. J. Umrigar (Cornell), Hong Jiang (Fritz Haber Institute), Amit Ghosal (IISER Calcutta), and H. U. Baranger (Duke).


12:03PM W24.00003 Iterative real-time path integral approach to nonequilibrium quantum transport, MICHAEL THORWART, Freiburg Institute for Advanced Studies, Univ. Freiburg, Germany, STEPHAN WEISS, Niels-Bohr-Institute, Univ. Copenhagen, Denmark, JENS ECKEL, REINHOLD EGGER, Institute for Theoretical Physics, Univ. Duesseldorf, Germany — We have developed a numerical approach to compute real-time path integral expressions for quantum transport problems out of equilibrium. The scheme is based on a deterministic iterative summation of the path integral (ISPI) for the generating function of the nonequilibrium current. Self-energies due to the leads, being non-local in time, are fully taken into account within a finite memory time, thereby including non-Markovian effects, and numerical results are extrapolated both to vanishing (Trotter) time discretization and to infinite memory time. This extrapolation scheme converges except at very low temperatures, and the results are then numerically exact. The method is applied to nonequilibrium transport through an Anderson dot. [1] S. Weiss, J. Eckel, M. Thorwart, and R. Egger, Phys. Rev. B 77, 195316 (2008).

12:15PM W24.00004 Time dependent transport in nanostructures1, KALMAN VARGA, Vanderbilt University — Using the Lagrange-function representation [1] we present time-dependent density functional calculations of the transport properties of nanostructures. To avoid the complications related to the semi-infinitive leads a complex absorbing potential (CAP) is added to the Hamiltonian [2,3]. This transformation leads to an effectively closed system which is computationally manageable. We will compare the results of the time dependent approach to those of time independent approaches for prototypical molecular devices such as benzene ring between gold electrodes and nanotubes.


1Supported by NSF ECS 0622146.
12:27PM W24.00005 Effective capacitance of small molecules and nanoscale devices in an electric circuit, XIAOGUANG ZHANG, Oak Ridge National Laboratory, JUN-QIANG LU, University of Puerto Rico-Mayaguez, SOKRATES PANTELIDES, Vanderbilt University — A quantum-mechanical-kinetic description of the capacitance of a molecule or nanodevice between two electrodes is complicated by the fact that one cannot unambiguously partition the electron density between the metal electrodes and the molecule or device. We introduce a procedure that leads to an unambiguous partitioning and to practical calculations using a linear response formalism for alternating current (AC) transport. The linear response theory is derived for a closed quantum system including the molecule and two electrodes with a finite length. The mutual capacitance between the two electrodes in the absence of a molecule or device is subtracted to obtain an effective capacitance for the molecule in the presence of the electrodes. Numerical calculations show that the effective capacitance converges with the increasing length of the electrodes. The converged results for small molecules of CO₂, CH₃, NH₃, H₂O, and benzene range from 0.18 to 2.832 (10⁻¹⁹ F).

1Work at CNMS at ORNL sponsored by Division of User Facilities, Office of Basic Energy Sciences, US Department of Energy.

12:39PM W24.00006 Theoretical Study of Electron Transport across Carbon Nanotube Junctions Decorated with Au Nanoparticles, KHOONGHONG KHOO, JAMES CHELIKOWSKY, University of Texas at Austin — In recent years, there has been extensive research on carbon nanotube networks owing to their potential for applications in transparent electronics, and several experimental studies have found that electrical conductivity across these networks can be increased by metal nanoparticle doping. To aid in understanding the mechanism of this conductance increase, we have performed first-principles calculations on nanotube junctions decorated with small Au nanoparticles. Our calculations show that the conductance of nanotube junctions is significantly increased by the introduction of odd-numbered Au nanoparticles, and electron transport is mediated by resonant tunneling through Au nanoparticle states. In addition, we find that interesting interference effects modulate conduction across doped nanotube junctions that connect near nanotube tips. This work was supported in part by NSF under DMR-0551195 and the U.S. Department of Energy under DE-FG02-06ER46286 and DE-FG02-06ER15760.

12:51PM W24.00007 Mechanism of Current-Induced Switching in Naphthalocyanine Molecular Device, TESFAYE ABTEW, NC State U. Raleigh NC, JERRY BERNHOLC, WENCHANG LU, NC State U. Raleigh NC and CSMD, ORNL, TN — Current-induced switching of inner cavity hydrogen atoms in a naphthalocyanine molecule has been reported experimentally [1]. The experiment shows a rotation of the lowest unoccupied molecular orbital (LUMO) image by 90° when the switching occurs. We study transport properties and energetics of a naphthalocyanine molecule sandwiched between gold leads using a parallel real space multigrid method. A non-equilibrium Green’s function formalism in a basis of optimized localized orbitals is employed to evaluate the current-voltage characteristics. Current-induced forces are evaluated and used to obtain bias-induced relaxations. The current-voltage characteristics indeed reveal contrasting high and low conductances depending on the orientation of the hydrogen atoms. However, a high energy barrier restrains the hydrogens from switching. We propose an alternative atomic configuration, which yields a much lower energy barrier for switching but still results in LUMO images that agree with the experimental results. [1] P. Liljeroth, J. Repp, and G. Meyer, Science 317, 1203 (2007).

1:03PM W24.00008 Negative differential resistance in molecular junctions: The effect of the electrodes electronic structure, NATALYA ZIMBOVSKAYA, University of Puerto Rico-Humacao, MARK PEDERSON, Naval Research Laboratory — We have carried out calculations of electron transport through a metal-molecule-metal junction with metal nanoclusters taking the part of electrodes. We show that negative differential resistance peaks could appear in the current-voltage curves. The peaks arise due to narrow features in the electron density of states of the metal clusters. The proposed analysis is based on the ab initio computations of the relevant wave functions and energies within the framework of the density functional theory using NRLMOL software package.

1 NZ acknowledges support from the ASEE and ONR Summer Faculty Research Program.

1:15PM W24.00009 Transport Properties of DNA Bases Placed in Graphene Nano-gap, CHRISTIAN WOLOWIEC, NICK KIOUSSIS, Department of Physics and Astronomy, California State University, Northridge, CA 91330, DMITRI NOVIKOV, Atomistic, Chief Technology Officer, Santa Clara, CA 95054 — There has been significant demand and research activity for the development of new DNA sequencing technologies employing transverse transport techniques. We present systematic first principles studies based on Density Functional Theory of the transport properties and current-voltage characteristics of nucleotide molecules of the DNA bases, placed in 1.2 nm gap formed between the zigzag edges of graphene-nano-electrodes. The linear dispersion of the graphene electrons and the local spin-polarization associated with the zigzag edges allow the exploration of both the charge- and spin-current signatures of the DNA bases to device properties. We present results in the tunneling regime of the charge- and spin-transport properties as the geometrical conformation of the bases is varied. Such signatures may be used experimentally for developing an efficient means of sequencing larger strands of DNA.

1 This research is supported by the National Science Foundation under grant No. PREM DMR-00116566.

1:27PM W24.00010 Quantum mechanical pseudopotential atomistic simulations of nanosized CMOS devices, LIN-WANG WANG, Lawrence Berkeley National Laboratory, XIANG-WEI JIANG, HUI-XIONG DENG, Semiconductor Institute, Chinese Academy of Science — We have used empirical pseudopotential to calculate the electronic structures of million atom CMOS systems. This is done by using the linear combination of bulk band (LCBB) method. For a nonequilibrium CMOS system with an applied source-drain bias, we have devised three different ways to calculate the inverse carrier charge densities and the corresponding currents. The first is to use partition functions extended from source and drain using their respective Fermi energies. The second is to use a spatially dependent local quasi-Fermi energy, and the third is to calculate the current using Bardeen’s tunneling current formula. In this talk, we will compare the results of these three different methods. We will also compare the quantum mechanical results with classical simulation results. This work was supported by U.S. Department of Energy under Contract No. DE-AC02-05CH11231. It has also been supported by Chinese National Natural Science Foundation.

1:39PM W24.00011 Nagaoka instabilities and coherent pairing in various cluster topologies, ARMEN KOCHARIAN, California State University, Los Angeles, GYANATH FERNANDO, Department of Physics, University of Connecticut, KALUM PALANDAGE, JAMES DAVENPORT, Computational Science Center, Brookhaven National Laboratory — Electron pairing and formation of various types of magnetic correlations in the ensemble of small clusters of different geometries are studied with emphasis on tetrahedron, square pyramid, etc under variation of interaction strength, electron doping and temperature. These exact calculations of charge and spin collective excitations and pseudogaps yield intriguing insights into level crossing phenomena and spatial interference, providing a new route to superconductivity in inhomogeneous HTSC systems, different from the BCS scenario. Phase diagrams resemble a number of inhomogeneous, coherent and incoherent nanoscale phases seen recently in high Tc cuprates, manganites and CMR nanomaterials.

1:51PM W24.00012 Calculation of complex band structure for low symmetry lattices\textsuperscript{1}, MANOJ SRIVASTAVA, Department of Physics, University of Florida, XIAOGUANG ZHANG, Oak Ridge National Laboratory, HAI-PING CHENG, Department of Physics, University of Florida — Complex band structure calculation is an integral part of a first-principles plane-wave based quantum transport method. \textsuperscript{1} The direction of decay for the complex wave vectors is also the transport direction. The existing algorithm \cite{1} has the limitation that it only allows the transport direction along a lattice vector perpendicular to the basal plane formed by two other lattice vectors, e.g., the c-axis of a tetragonal lattice. We generalize this algorithm to nonorthogonal lattices with transport direction not aligned with any lattice vector. We show that this generalization leads to changes in the boundary conditions and the Schrödinger's equation projected to the transport direction. We present, as an example, the calculation of the complex band structure of fcc Cu along a direction perpendicular to the (111) basal plane. \cite{1} Hyoun Joon Choi and Jisoon Ihm, Phys. Rev. B 59, 2267 (1999).

2:03PM W24.00013 Reduced Bloch mode expansion for fast band structure calculations, MAHMOUD HUSSEIN, University of Colorado at Boulder — In this paper, we present reduced Bloch mode expansion for fast band structure calculations in lattice dynamics. The expansion employs a natural basis composed of a selected reduced set of Bloch eigenfunctions. The reduced basis is selected within the irreducible Brillouin zone at high symmetry points determined by the medium's crystal structure and group theory. At each of the reciprocal lattice section points, a number of Bloch eigenfunctions are used to accurately represent the dispersion relations. The resulting reduced Bloch mode expansion greatly improves both the memory and computational time required for band structure calculations.


11:15AM W25.00001 Atomically Flat Graphene on Mica Substrates, LI LUI, CHUN HUNG LUI, KIN FAI MAK, GEORGE FLYNN, TONY HEINZ, DEPARTMENT OF PHYSICS, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 COLLABORATION, DEPARTMENT OF CHEMISTRY, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 COLLABORATION — Much recent interest has focused on the question of the intrinsic flatness of monolayers of exfoliated graphene. In studies of both suspended graphene [Meyer et al, Nature 446 (2007)] and graphene deposited on SiO\textsubscript{2} substrates [Stolyarova et al, PNAS 104 (2007)], graphene monolayers exhibited clear variations in height. For suspended films, this variation was attributed to an intrinsic rippling instability [Meyer et al, Nature 446 (2007)]. In the case of graphene on SiO\textsubscript{2} substrates, the role of intrinsic and substrate-induced effects remained unclear because of the corrugation of the substrate. In this paper we present results of a detailed study of the morphology of exfoliated graphene monolayers deposited on the atomically flat terraces of cleaved mica surfaces. Using high-resolution atomic force microscopy (AFM), we demonstrate that graphene monolayers on mica, when measured with lateral spatial resolution of \(\sim\) 6nm, are flat to over micron lateral length scales to within the instrumental sensitivity of 50 pm. These results stand in sharp contrast to the behavior reported for both suspended graphene and graphene on SiO\textsubscript{2} substrates.

11:27AM W25.00002 Scattering in monolayer graphene on SiO\textsubscript{2} observed by STS, APARNA DESHPANDE, BRIAN LEROY, University of Arizona, WENZHONG BAO, FENG MIAO, CHUN NING LAU, University of California Riverside — The intrinsic ripples of graphene and its distinctive band structure make graphene a novel two-dimensional system of interest for the study of structural and electronic properties. To probe the influence of graphene structure on its electronic properties we have carried out scanning tunneling spectroscopy (STS) measurements on exfoliated graphene on SiO\textsubscript{2} with an ultra high vacuum scanning tunneling microscope (UHV STM) at 4.2 K. Atomically resolved local density of states (LDOS) images show an interference pattern due to scattering. 2D Fourier transforms of the LDOS maps reveal two types of scattering wave vectors corresponding to long range intravalley scattering and short range intervalley scattering. Interv valley scattering due to short range potential variations leads to a \(\sqrt{3}\times\sqrt{3}\) R30\textdegree interference pattern in the LDOS while intravalley scattering causes long range disorder in the LDOS images. Our measurements present a comprehensive picture of scattering mechanisms in exfoliated graphene and underline the contribution of random impurities, defects and SiO\textsubscript{2} morphology to the electronic properties of graphene.

11:39AM W25.00003 STM on Gate-Tunable Graphene, YUANBO ZHANG, Dept. of Physics, UC Berkeley — We have successfully performed atomically-resolved scanning tunneling microscopy and spectroscopy (STS) on mechanically exfoliated graphene samples having tunable back-gates. We have discovered that the tunneling spectra of graphene flakes display an unexpected gap-like feature that is pinned to the Fermi level for different gate voltages, and which coexists with another depression in density-of-states that moves with gate voltage. Extensive tests and careful analysis show that the gap-feature is due to phonon-assisted inelastic tunneling, and the depression directly marks the location of the graphene Dirac point. Using tunneling spectroscopy as a new tool, we further probe the local energetic variations of the graphene charge neutral point (Dirac point) to map out spatial electron density inhomogeneities in graphene. Such measurements are two orders of magnitude higher in resolution than previous experiments, and they can be directly correlated with nanometer scale topographic features. Based on our observation of energy-dependent periodic electronic interference patterns, our measurements also reveal the nature of impurity scattering of Dirac fermions in graphene. These results are significant for understanding the sources of electron density inhomogeneity and electron scattering in graphene, and the microscopic causes of graphene electron mobility.

12:15PM W25.00004 Effect of disorder on electron tunneling in graphene layers through potential barriers, VRINDA THAREJA, MANISH SHARMA, SANKALPA GHOSH, Indian Institute of Technology Delhi — Electrons at the fermi level in Graphene monolayer behave like massless Dirac fermions. Using a coherent potential approximation, we study the tunneling of such electrons through a double barrier potential in presence of disorder. We subsequently extend this study in the case of periodic lattice potentials. Our approach involves using the Green's function calculation and is particularly amenable to studying the effect of disorder, impurities and defects on electron propagation through Graphene.

12:27PM W25.00005 Scanning Gate Microscopy on Patterned Graphene Nanoribbons, ANDREI GARCIA, MARKUS KOENIG, KATHRYN TODD, DAVID GOLDBABER-GORDON, Stanford University — Graphene-based electronic devices are of interest due to the unique nature of the graphene band structure. Bulk graphene exhibits a gapless linear dispersion near the Fermi level. When graphene is etched to form a narrow ribbon a transport gap opens at the Dirac point. The origin of this transport gap in patterned graphene nanoribbons remains an unresolved problem. Two possible explanations for the origins of the gap are confinement in the direction perpendicular to the length of the ribbon and localization due to disorder along imperfectly formed ribbon edges. We explore the local properties of this gap in nanoribbons using a scanning gate microscope.
12:39PM W25.00006 Scanning tunneling microscopic (STM) studies of strain-induced local density of states modulations in single-layer graphene on SiO₂  A.P. LAI, M.L. TEAGUE, C.R. HUGHES, A.D. BEYER, N.-C. YEH, M.W. BOCKRATH, Phys. Dept, Caltech, Pasadena, CA, J. VELASCO, C.N. LAU, UC Riverside — We report strain-induced spatial modulations in the electronic density of states (DOS) of single-layer graphene on SiO₂. Spatially resolved topographic and spectroscopic measurements were performed simultaneously at 77 K and at pressures < 10⁻⁷ torr. Fourier transformation of local topography shows a distorted hexagon with lattice vectors ranging from a₀=3.0 ±0.2 Å to 2.1±0.2 Å as the result of surface corrugation from the roughness of the underlying substrate. A spatially varying strain map derived from local distortions of the lattice constants correlates well with the surface topography. Strained graphene, due to three dimensional surface corrugations of ± 5 Å over 10 nm lateral distance, show parabolic “U-shaped” conductance vs. biased voltage spectra rather than the Dirac-like “V-shaped” spectra. In contrast, for regions of relaxed graphene, Dirac-like spectra are recovered. The Dirac voltage, V_D, determined from the biased voltage of conductance minimum, appears to be position independent at V_D=36±5 meV, while the minimum conductance and the degree of derivation from the Dirac-like spectra at low energies appear to correlate directly with the topography. This work was supported by NSF/NRI under Caltech/CSEM.

12:51PM W25.00007 SPM measurements of graphene corrugation and spatial correlation  WILLIAM CULLEN, JIANHAO CHEN, University of Maryland, MASA ISHIGAMI, University of Central Florida, ELLLEN WILLIAMS, MICHAEL FUHRER, University of Maryland — In order to determine the effect of graphene corrugation on electronic transport, it is most important to know the spatial correlation properties of the corrugated graphene structure. In spite of much experimental effort, there is still contentious debate about the structure of graphene, both in supported and suspended geometries. It has frequently been asserted that a graphene monolayer exfoliated onto a SiO₂ substrate may display “intrinsic” corrugation — rippled structure which is not derived from the topography of the underlying substrate. Here, we report recent UHV NC-AFM and STM results which show that anomalous corrugation may be observed due to local interaction between the tip and the graphene monolayer. Our results show that non-perturbative NC-AFM measurement reveals a graphene topography which is as smooth as the underlying SiO₂, with height-height correlation exponent H=1. STM measurement of graphene, due to uncontrollable tip-sample forces, may exhibit anomalous corrugation depending on tip condition.

1Supported by a NRI supplement to the UMD-NSF-MBSEC grant #DMR 0520471.
2:03PM W25.00013 Enhancement of nearest neighbor spin-singlet correlations in d-wave SNS graphene Josephson junctions, ANNICA BLACK-SCHAFER, SEBASTIAN DONIACH, Stanford University — Using the self-consistent tight-binding Bogoliubov-de Gennes (BdG) formalism we investigate the effect of nearest neighbor spin-singlet bond (SB) correlations in a graphene SNS Josephson junction with d-wave superconducting contacts. All pi-bonded planar organic molecules, of which graphene is the infinite extension, show a preference for SB over polar configurations, as originally captured by Pauling’s idea of resonating valence bonds. At strong enough coupling and/or high doping levels, these correlations will give rise to a d-wave superconducting state. However, the estimated coupling strength in graphene would require a doping level not currently experimentally achievable by a gating bias. We demonstrate that by creating a graphene SNS Josephson junction with d-wave contacts, for example by depositing a high-Tc cuprate on top of the graphene, it should be possible to enhance the effect of the SB correlations and see clear signatures of d-wave pairing in proximity effect, superconducting decay length, and supercurrent.

Thursday, March 19, 2009 11:15AM - 2:15PM –
Session W26 DMP: Focus Session: Graphene XVI: Functionalization and Growth I

11:15AM W26.00001 Impact of Atomic Hydrogen Adsorption on Transport Properties of Graphene, JYOTTI KATOCH, Department of Physics, University of Central Florida, JIANHAO CHEN, Dept of Physics, Center for Nanophysics and Advanced Materials, and Materials Research Science and Engineering Center, Unive. of Maryland, College Park, MASA ISHIGAMI, Department of Physics, University of Central Florida — We have measured transport properties of graphene as a function of surface coverage by atomic hydrogen in ultra high vacuum. Hydrogen adsorption is reversible at moderate temperatures and alters electronic properties of graphene at atomic scale. We will discuss dependence of minimum conductivity and field-effect carrier mobility on the density of adsorbed hydrogen.

11:27AM W26.00002 Determination of the Crystallographic Orientation of Graphene by Raman Spectroscopy, MINGYUAN HUANG, Department of Mechanical Engineering, Columbia University, HUGEN YAN, Department of Physics and Electrical Engineering, Columbia University, CHANGYAO CHEN, Department of Mechanical Engineering, Columbia University, DAOHUA SONG, TONY HEINZ, Department of Physics and Electrical Engineering, Columbia University, JAMES HONE, Department of Mechanical Engineering, Columbia University — We present a systematic study of the Raman spectra of the G band in graphene monolayers under tunable uniaxial tensile stress. The G band splits into two distinct sub-bands; G+ and G−. The polarization dependence that reflects the angle between the axis of the stress and the underlying graphene crystal axes. Polarized Raman spectroscopy therefore constitutes a purely optical method for the determination of the crystallographic orientation of graphene.

11:39AM W26.00003 Growth and Characterization of CVD Graphene, ALFONSO REINA, XIAOTING JIA, JOHN HO, DANIEL NEZICH, HYUNGBIN SON, VLADIMIR BULOVIC, MILDRED S. DRESSELHAUS, JING KONG, Massachusetts Institute of Technology — Large-area (~cm²) graphene films are grown by ambient pressure chemical vapor deposition (CVD) on evaporated Ni films. We show that proper engineering of the Ni film properties, such as grain structure and surface roughness, and the use of ultra-diluted hydrocarbon flow yields films consisting of 1 to ~10 graphene layers in thickness. Furthermore, the produced graphene can be transferred, by wet-etching the underlying Ni, to a variety of substrates allowing graphene coverage over large areas on different materials such as glass, polymers or other semiconductors. Raman Spectroscopy, electron diffraction and transmission electron microscopy suggest disordered stacking of regions with multilayer graphene. Growth mechanisms will also be discussed. Opto-electronic properties and ambipolar transfer characteristics of the produced material is also demonstrated.

11:51AM W26.00004 Chemical exfoliation procedure for graphene deposition1, MICHELLE ZIMMERMANN, MAHITO YAMAMOTO, BRAD CONRAD, JIANHAO CHEN, ELLEN WILLIAMS, Department of Physics and University of Maryland Materials Research Science and Engineering Center, University of Maryland, College Park, MD 20742 — Mechanical exfoliation techniques for graphene production yield flakes which are too small and too rare for feasible large-scale experiments or commercial device fabrication. We present a systematic evaluation of the steps involved in chemical exfoliation of graphite to generate suspended graphene sheets. The approach is based on the solubilizing of a graphite intercalation compound in a polar solvent, analogous to solubilization of CNT salts [1] and recently reported for graphene [2]. A shift in the Raman G peak of graphite provides a metric of the degree of intercalation of lithium and naphthalene into graphite flakes. To optimize deposition onto SiO2 substrates, we compare drop casting, spin-coating and dip-coating, as well as the effects of different surface treatments (UV ozone, oxygen plasma, functionalization). [1] A. Pécaut, et al., J. Am. Chem. Soc. 127, 8 (2005). [2] C. Vallès, et al., J. Am. Chem. Soc. 130, 15802 (2008).

1Supported by NSF Grant No. DMR-080976 and UMD-NSF-MRSEC-SEF.

12:03PM W26.00005 Anomalously high conductivity in bromine-intercalated graphite, A.F. HEBARD, S. TONGAY, J. HVANG, D.B. TANNER, D. MASLOV, University of Florida — We have found that when graphite is intercalated with bromine, the ab-plane (~c-axis) conductivity sharply increases (decreases). Characterization of the Br intercalated samples by exposure time, weight uptake, sputter Auger spectroscopy and X-ray diffraction show a Br concentration that is uniformly distributed within a graphite host having an expanded interplanar spacing dc. The ab-plane conductivity is enhanced by several orders of magnitude in the temperature range from 300 K down to 1.7 K and shows no sign of saturation with increasing Br concentration. Hall measurements confirm a pronounced increase in the density of negative carriers consistent with an increased optical reflectivity (below 3000 cm⁻¹). The inferred plasma frequencies and extrapolated dc conductivities are consistent with the transport measurements. The diamagnetic susceptibility decreases with increasing Br concentration and follows a temperature dependence from which a Fermi energy that increases with increasing Br concentration is extracted. By increasing dc, the ab-plane conductivity of Br intercalated graphite begins to resemble the additive contributions of parallel connected doped graphene sheets and thus has implications for carbon based electronics.

1Work supported by NSF #DMR-0704240 and DOE #DE-FG02-OLER45984.

12:15PM W26.00006 Influence of substrates on graphene layers: Raman study1, JORGE CAMACHO, LIYUAN ZHANG, TONY VALLA, IGOR ZALIZNYAK, Brookhaven National Laboratory — Electrical contacts and a substrate can significantly influence electronic and physical properties of graphene. Charge transfer, strain, introduction of various impurities and defects are some of the factors that can alter graphene properties. Therefore, the graphene has been considered in any real graphene-based device. Here we use Raman spectroscopy to study effects of different substrates and adsorbates on graphene Raman-active modes. We find that the intensity, frequency and line-width of some modes are very sensitive to the chemical environment of graphene sheets, reflecting the changes in interactions of these modes with charge carriers and degree of disorder introduced in the system.

1This work was supported by the US Department of Energy.
Doping effect of electrode on Graphene\textsuperscript{1}, KEYU PI, KATHY MCCREARY, WEI HAN, YAN LI, WENZHONG BAO, CHUN NING LAU, ROLAND KAWAKAMI, University of California, Riverside. ROLAND, KAWAKAMI TEAM, CHUN-NING, LAU COLLABORATION — Graphene as a carrier tunable transport media has drawn a lot of interest since its discovery. It has recently been reported that invasive electrode contacts cause electron-hole asymmetry\textsuperscript{1} which will affect the transport properties. To study this effect, we developed an in-situ measurement system that combines Molecular Beam Epitaxy (MBE) with transport measurement. Fine control of the material deposition rate allows us to study the doping effect on graphene at the early stages of electrode formation.\textsuperscript{1}\textsuperscript{1} B. Huard et al., PRB. 78. 121402(R), 2008

We acknowledge the support of ONR, NSF and CNID.

Multi-layer graphene derived from graphite fluoride, S.H. CHENG, K. ZOU, A. GUPTA, H.R. GUTIERREZ, P. EKLUND, J.O. SOFO, J. ZHU, Department of Physics, The Pennsylvania State University, F. OKINO, Department of Chemistry, Faculty of Textile Science and Technology, Shinshu University — We produce multi-layer graphene through the reduction of graphene fluoride. Graphite fluoride (CF) is synthesized by reacting F\textsubscript{2} with graphite at 500 - 600°C. We obtain few-layer CF sheets through mechanical exfoliation and characterize their properties with electron diffraction, TEM, AFM, Raman and transport measurements. Electron diffraction spectra of fluorinated few-layer CF show the persistence of six-fold hexagonal symmetry and long-range in-plane crystalline order. Domains of varying thickness in both AFM and TEM measurements suggest an incomplete fluorination. Raman spectra of few-layer CF show the appearance of a D band (\textsim\sim 1350 cm\textsuperscript{-1}) as expected from sp\textsuperscript{2} bonding. Few-layer CF sheets are defluorinated in flowing H\textsubscript{2}/Ar (10%/90%) at 500 - 600°C. AFM studies of defluorinated CF show a pronounced decrease in roughness and thickness, suggesting the removal of fluorine. Raman spectra of defluorinated CF show a reduced background with an enhanced 2D peak (\textsim\sim 2700 cm\textsuperscript{-1}). We present transport measurements in field effect transistors fabricated from CF and defluorinated sheets and compare with that of pristine graphene and graphene-oxide reduced graphene.

Size Selection of Metal Nanoparticles on Few Layer Graphene\textsuperscript{1}, LUKE A. SOMERS, ZHENGTANG Luo, E.J. MELE, A.T. CHARLIE JOHNSON, University of Pennsylvania — We find layer number dependence in the size of metal nanoparticles grown on 1 to 10 layer graphene. Graphene is an attractive substrate for investigating and using nanoparticles due to its loose interaction with them. To preserve this condition it is ideal to grow particles in place rather than deposit them from solution. We find that annealing of evaporated metal nanoparticles on graphene and few layer graphene surfaces tightens their size distribution. The number of graphene layers changes the selected size. These results are in quantitative agreement with a model incorporating surface, bulk, and coulomb free energies.

This work was supported by the JSTO DTRA and the Army Research Office Grant # W911NF-06-1-0462.

Optimization of high quality epitaxial graphene growth on SiC, MING RUAN, MICHAEL SPRINKLE, YIKE HU, CLAIRE BERGER, WALTER DE HEER, Georgia Institute of Technology — We have developed an RF inductance furnace to grow epitaxial graphene(EG) of very high quality on SiC. EG has attracted much attention during the past years due to its potential as next generation material for electronic devices. The formation of graphene on silicon carbide by sublimation of Si is a complicated process that is not well understood yet. We present here our latest result on the growth of epitaxial graphene in low vacuum. The research is carried out for multilayer graphene growth on 4H SiC (000\textbar). Surface free energies of the monolayers and the SiO\textsubscript{2} (CF) is synthesized by reacting F\textsubscript{2} with graphite at 500 - 600°C. We obtain few-layer CF sheets through mechanical exfoliation and find that surface diffusion promotes a rough morphology. To reduce the mobility of surface atoms, the graphene surface is dressed by Ti atoms prior to MgO deposition. With as little as 0.5 ML monolayer of Ti, the MgO overlayer becomes atomically smooth. Single layer graphene on graphene by molecular beam epitaxy and find that surface diffusion promotes a rough morphology. To reduce the mobility of surface atoms, the graphene layers, such as MgO, are often used to minimize the conductivity mismatch between graphene and electronic contacts. We investigate the growth of MgO films on graphene by molecular beam epitaxy and find that surface diffusion promotes a rough morphology. To reduce the mobility of surface atoms, the graphene surface is dressed by Ti atoms prior to MgO deposition. With as little as 0.5 ML monolayer of Ti, the MgO overlayer becomes atomically smooth. Single layer graphene has been patterned into nanoscale devices to study the effect of the Ti dressing layer and MgO overlayer on the electronic and spintronic properties.

Size Selection of Metal Nanoparticles on Few Layer Graphene\textsuperscript{1}, LUKE A. SOMERS, ZHENGTANG Luo, E.J. MELE, A.T. CHARLIE JOHNSON, University of Pennsylvania — We find layer number dependence in the size of metal nanoparticles grown on 1 to 10 layer graphene. Graphene is an attractive substrate for investigating and using nanoparticles due to its loose interaction with them. To preserve this condition it is ideal to grow particles in place rather than deposit them from solution. We find that annealing of evaporated metal nanoparticles on graphene and few layer graphene surfaces tightens their size distribution. The number of graphene layers changes the selected size. These results are in quantitative agreement with a model incorporating surface, bulk, and coulomb free energies.

1:03PM W26.00010 Growth of atomically smooth MgO films on graphene by molecular beam epitaxy.\textsuperscript{1} — KATHLEEN MCCREARY, University of California, Riverside, WEI HAN, WEI-HUA WANG, KEYU PI, WENZHONG BAO, FENG MIAO, ROLAND KAWAKAMI, CHUN-NING LAU, UCR — Graphene has been the focus of many recent studies involving both electronic and spintronic devices due to its tunable charge carriers, high mobility, and possibility of long spin coherence lifetimes. To improve the spin injection into graphene spintronic devices, dielectric layers, such as MgO, are often used to minimize the conductivity mismatch between graphene and electronic contacts. We investigate the growth of MgO films on graphene by molecular beam epitaxy and find that surface diffusion promotes a rough morphology. To reduce the mobility of surface atoms, the graphene surface is dressed by Ti atoms prior to MgO deposition. With as little as 0.5 ML monolayer of Ti, the MgO overlayer becomes atomically smooth. Single layer graphene has been patterned into nanoscale devices to study the effect of the Ti dressing layer and MgO overlayer on the electronic and spintronic properties.

Growing Epitaxial Graphene on an Insulator by MBE, CHANDRA MOHAPATRA, JAMES ECKSTEIN, Department of Physics, University of Illinois Urbana Champaign, USA — We have used electron beam evaporation of solid carbon (C) to deposit graphene on MgO <111> at 850°C. The growth appears epitaxial as observed by in-situ RHEED which also reveals that the hot scattering surface transitions from an insulator to a conductor after deposition of 1 monolayer of C. Growth at higher temperatures gives better crystallinity. We further characterize the film by ex-situ Raman spectroscopy, AFM and transport. Raman reveals all the characteristic G, D and 2D peaks of graphene and the 2D peak can be fit to a single lorentzian typical for graphene. AFM pictures show that the surface consists of flat connected domains, which are uniform across the substrate. Electrical transport shows insulating behavior with resistance (R) varying as 1/T\textsuperscript{2}. This work was supported by the DOE BES at the F. Seitz Materials Research Laboratory at the University of Illinois, Urbana.

The effect of self-assembled monolayers on graphene conductivity and morphology, T. L. MOORE, J. H. CHEN, B. RIDDICK, E. D. WILLIAMS\textsuperscript{1}, University of Maryland, College Park — Graphene transport properties are limited by charge defects in SiO\textsubscript{2}, and by large charge density due to strong interaction with SiC. To modify these effects we have treated 300 nm SiO\textsubscript{2} with trichlorosilanes with different termination groups including pure and fluoro and amino-terminated hydrocarbons for use as substrates for mechanical exfoliation of graphene. XPS measurements verify the presence of the expected termination groups. AFM measurements reveal modified monolayer roughness and correlation lengths; for a fluorinated carbon chain the RMS roughness is 0.266 ± 0.017 nm and the correlation length is 10.2 ± 0.7 nm compared to 0.187 ± 0.011 nm and 19.8 ± 2.5 nm for SiO\textsubscript{2}. Surface free energies of the monolayers and the SiO\textsubscript{2} blank have been computed from static contact angle measurements and all decrease the SiO\textsubscript{2} surface free energy; for the fluorinated carbon chain monolayer a decrease of 20 mJ/m\textsuperscript{2} from SiO\textsubscript{2}. We will discuss the ease of exfoliation, and the morphology and conductivity of graphene on these monolayers.

\textsuperscript{1}Supported by the MRSEC University of Maryland.
The effect of SiO$_2$ surface states on the electronic characteristics of graphene FET devices

Jorge Sofo, Ning Shen, Hugo Romero, Peter Eklund, Dept. of Physics, Penn State — Electronic states localized at the surface of oxide semiconductors are a common cause of their low ionization potential. We study the properties of the SiO$_2$ surface states using density functional theory (DFT) and show that they strongly affect the intrinsic doping of graphene on oxidized silicon substrates. We present simple empirical model that it is parameterized from the DFT calculations. The model demonstrates that Dirac voltages as large as 50 V and intrinsic n-doping are produced by the presence of these surface states. We extend it to include the effect of other adsorbates, such as water, that modify the dielectric properties of the device.

Efficient manipulation of zigzag and armchair edges in graphene nanoribbons by joule heating

Xiaoting Jia, Mario Hofmann, Vincent Meunier, Bobby Sumpter, Jessica Campos-Delgado, Jose Romo-Herrera, Hyungbin Son, Ya-Ping Hsieh, Alfonso Reina, Jieing Kong, Mauricio Terrones, Mildred Dresselhaus — Edge study in graphene nanoribbons has attracted lots of interest in recent years, due to the different electronic properties of the ribbons arising from zigzag and armchair edges. Here we demonstrate and monitor an efficient crystallization process for graphite nanoribbon edges by Joule heating inside an integrated transmission electron microscope (TEM) equipped with a scanning tunneling stage STM (TEM-STM system). With this system we were able to produce for the first time atomically smooth zigzag or armchair edges from defective rough edges present in graphite nanoribbons, by applying a controlled voltage, while observing the structural behavior in-situ. Edge motion along certain preferred crystallographic orientations is observed, and the transformational effects of Joule heating and applied electric field are described. This work demonstrates both the possibility of self-eliminating lattice defects by applying a bias voltage, and an effective way to produce clean zigzag and armchair edges, which could be useful for both fundamental studies of edge reactivity, magnetism and the development of future electronics applications.


Functionalized Heterofullerenes for Hydrogen Storage

Puru Jena, Qian Wang, Virginia Commonwealth University, Qiang Sun, Peking University and Virginia Commonwealth University — Using density functional theory we show that Li decorated B doped heterofullerene (Li12C48B12) has the desired properties of a hydrogen storage material: (1) The Li atoms remain isolated. (2) Through charge transfer to electron deficient C48B12 heterofullerene, the Li atoms become positively charged. (3) Each Li atom is able to bind up to three H2 molecules which remain in molecular form, and the binding energies of successive H2 molecules are in the range of 0.135 to 0.172 eV/H2, suitable for ambient temperature storage; (4) The gravimetric density reaches the 9 wt.% limit necessary for applications in the mobile industry.

Can Silicon Carbide Nanotubes Be Effective Storage Medium for Hydrogen Storage

Souptik Mukherjee, Asok Ray, UTA — A systematic study of molecular hydrogen adsorption on three different atomic configurations of armchair SiCNTs has been performed. In the first stage of our study, first principles calculations using both density functional theory (DFT) and hybrid density functional theory (HDFT) as well as the finite cluster approximation have been performed to study the adsorption of molecular hydrogen on three types of armchair (9, 9) silicon carbide nanotubes. The distances of molecular hydrogen from the outer wall of the nanotubes have been optimized manually using the B3LYP and PW91 functionals and results have been compared in detail with published literature results. In the second part of our study, hydrogen molecule has been adsorbed from both inside as well as from the outer wall of nanotubes ranging from (3, 3) to (6, 6) for all three types. A detailed comparison of the binding energies, equilibrium positions and Mulliken charges has been performed for all three types of nanotubes and for all possible sites in those nanotubes. In the third phase, co-adsorption of two hydrogen molecules has been carried out. Possibilities of hydrogen storage have been explored in detail.

Nanostructured Adsorbents for Hydrogen Storage

Lin Simpson, National Renewable Energy Laboratory — To meet the DOE goals for hydrogen storage, NREL and our partners have focused development efforts on the use of nanomaterials with hydrogen binding energies between ~4 and 40 kJ/mol. The use of these types of materials enables hydrogen to be reversibly adsorption/desorption with moderate to low temperatures and pressures, and greatly simplifies the refueling/regeneration process. NREL is investigating multiple approaches to obtain high hydrogen sorption materials with the common goal of determining the underlying mechanisms and applying a fundamental basis to intelligently design advanced materials. NREL will provide detailed hydrogen capacity/performance and reproducible processing information for promising nanostructured materials. This will include detailing the potential for hydrogen storage by nanostructures, the effects of dopants, demonstrate materials with greater than 4 wt% hydrogen uptake, and discuss the potential to develop materials with 9 wt% or more hydrogen storage.

A comparative investigation of H$_2$ adsorption energy in Cd- and Zn-based metal organic framework-5

Pornjuk Srepusharawoot, Condensed Matter Theory Group, Dept. of Physics and Materials Science, Uppsala University, Sweden; Dept. of Physics, Khon Kaen University, Thailand. Carlos Moyses Araujo, Andeas Blomqvist, Ralph Scheicher, CMT Group, Uppsala; Rajeev Ahuja, CMT Group, Uppsala; Applied Materials Physics, Dept. of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — Density functional theory has been used to study the physisorption energies of hydrogen at all possible adsorption sites near the metal oxide cluster in both Cd- and Zn-based Metal Organic Framework-5 (MOF-5). Three types of exchange-correlation functionals (LDA, GGA-PW91, and GGA-PBE) were compared. The binding for all adsorption sites in Cd-based MOF-5 was found to be generally stronger than in Zn-based MOF-5. In particular, the hydrogen adsorption energy at the secondary adsorption sites of Cd-based MOF-5 is increased by about 25% compared to Zn-based MOF-5. This result suggests that Cd-based MOF-5 might be better suited to store hydrogen at a given temperature than Zn-based MOF-5. See also: J. Chem. Phys. 129, 164104 (2008).
12:03PM W27.00005 Design of Multi-Decker Incorporated Metal Organic Frameworks for Hydrogen Storage. KIRAN BOGAVARAPU, McNeese State University, ANIL KANDALAM, McNeese State University — Metal Organic Frameworks (MOFs) are a new class of rationally designed microporous hybrid (organic-inorganic) materials. They have recently gained attention as potential hydrogen storage systems with gravimetric density meeting the DOE 2015 targets of 9 wt%. However, due to weak interaction between the molecular hydrogen and the host MOF (see figure), high pressures are required to reach the target storage levels. Recently, multi-decker organometallic complexes are shown to exhibit the ideal thermodynamics and kinetics for hydrogen storage. However, it is not clear if these multi-decker complexes can retain their hydrogen storage capability when assembled into a bulk-material. In this presentation, we investigate the hydrogen storage capability of a new class of materials by combining the strengths of MOFs and decker complexes. An ideal way to integrate these two systems is to incorporate the multi-deckers into the structural framework of MOFs. In these hybrid materials, the multi-decker units are expected to maintain their structural integrity and thereby retain the hydrogen storage capacity with an added advantage of being a part of stable porous MOF back-bone.

12:15PM W27.00006 Hydrogen Adsorption by High Surface Area Micro-porous Carbon Synthesized from Phenol-Formaldehyde. QINGYUAN HU,1 Purdue University, GREGORY P. MEISNER, GM Research and Development Center — A high surface area microporous carbon material can be synthesized by mixing the activation reagent potassium hydroxide into a carbon precursor solution of phenol-formaldehyde oligomers. Some polymerization of the carbon precursor occurs during the initial mixing, and further polymerization is completed by heating to 160°C. Carbonization and activation is accomplished by heating to 500°C - 900°C in an inert atmosphere. The porosity and surface area of the resulting carbon material depends predominantly on the amount of activation reagent added to the carbon precursor solution and the carbonization/activation temperature and time. Optimized synthesis conditions yield a microporous carbon with a very high BET specific surface area of nearly 3000 m²/g and a narrow pore size distribution. This new synthesis approach yields surface areas dramatically larger than those typically obtained by traditional chemical activation methods for porous carbon where solid carbon precursors are soaked in activation reagent solutions. Hydrogen adsorption up to 5.75 wt% at 77 K and above 20 bars hydrogen pressure is observed for this new microporous carbon material.

12:27PM W27.00007 Ab-initio study of hydrogen storage of Titanium-decorated organic systems with hydroxyl groups. MANH CUONG NGUYEN, JISOON IHM, Department of Physics and Astronomy, Seoul National University — Using first-principles calculation, we study hydrogen storage of Titanium-decorated organic systems with hydroxyl groups, such as propane-1,3-diol. The results show that Ti atom is bound selectively to hydroxyl groups with the binding energy of 3.0 eV. The first hydrogen molecule adsorbed on Ti is dissociated and then Ti can bind three hydrogen molecules in molecular form more with the binding energy suitable for reversible processes (adsorption and desorption) in hydrogen storage at ambient temperature and pressure. Using thermodynamics, the usable number of hydrogen molecules per Ti atom is almost three due to the proper binding energy of the last three hydrogen molecules on Ti. Based on this result, we can design organic systems with hydroxyl groups to store hydrogen with the reduction of the tendency of transition metal clustering. We also explain the mechanism of multi-container hydrogen adsorption on Ti by generalizing the Kubas model.

12:39PM W27.00008 First-principles study of dihydrogen interaction of porphyrin-like nitrogen-doped graphenes. WOON IH CHOI, National Renewable Energy Laboratory, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, YONG-HYUN KIM, National Renewable Energy Laboratory — We have studied electronic structure and dihydrogen (H2) binding characteristics of porphyrin-like nitrogen-doped graphenes (PNGs) by performing first-principles total energy calculations based on the density functional theory. The stability of PNGs and the H2 binding ability of the PNG metal centers (Ca and 3d transition metals from Sc to Zn) have been analyzed within the generalized gradient approximation. We have found that Ca, Sc, Ti, Co, and Ni can be incorporated relatively easily into the nitrogen-doped graphenes, while V, Fe, Cu, and Zn are less likely to be. The PNGs can be used for active building blocks of hydrogen storing metal-organic frameworks. Due to the unique crystal field splitting of the planar PNGs, approaching dihydrogen exclusively interacts with the dz2 orbitals of the core metals. We also found that intra-/inter-orbital charge transfer plays a key role in the dihydrogen binding. Finally, we will discuss how such dihydrogen binding can be modified by external strain.

12:51PM W27.00009 Magnetic Properties of High-Surface-Area Carbons and Their Effect on Adsorbed Hydrogen. JIMMY ROMANOS, MATTHEW BECKNER, MICHAEL KRAUS, JACOB BURRESS, PETER PFEIFER, Dept. of Physics and Astronomy, Univ. of Missouri — We report the discovery that a large number of nanoporous carbon samples, made from corn cob and exhibiting high hydrogen storage capacities (Pfeifer et al, Mater. Res. Soc. Symp. Proc. 1041 R02-02 (2008)), show unexpected magnetic properties, due to iron impurities in the samples. Magnetization curves are consistent with ferromagnetic and/or super-paramagnetic behavior. Magnetic susceptibilities, saturation magnetizations, coercivities and remanence magnetizations, from measurements on a SQUID magnetometer, will be presented, and their temperature dependence will be discussed. Results will be presented regarding the presence of small iron clusters, magnetic properties of iron-leached samples, and hydrogen binding energies as a function of iron leaching. This material is based on work supported by the U.S. Department of Energy under Award No. DE-FG-08GO18142.

1:03PM W27.00010 Boron-Doped Carbon Nanospaces for High-Capacity Hydrogen Storage. MATTHEW BECKNER, JACOB BURRESS, CARLOS WEXLER, PETER PFEIFER, Dept. of Physics and Astronomy, Univ. of Missouri — The Alliance for Collaborative Research in Alternative Fuel Technology (ALL-CRAFT, http://all-craft.missouri.edu) has been optimizing high surface area (>3,000 m²/g) activated carbon nanospaces for high capacity hydrogen storage. Boron-doped samples have been produced using solid, liquid, and vapor phase boron doping. The boron-doped samples were shown by using x-ray diffraction and nitrogen adsorption that boron-doping increases the density functional theory results of nitrogen-doped graphenes, while V, Fe, Cu, and Zn are less likely to be. The PNGs can be used for active building blocks of hydrogen storing metal-organic frameworks. Due to the unique crystal field splitting of the planar PNGs, approaching dihydrogen exclusively interacts with the dz2 orbitals of the core metals. We also found that intra-/inter-orbital charge transfer plays a key role in the dihydrogen binding. Finally, we will discuss how such dihydrogen binding can be modified by external strain.

1:15PM W27.00011 Hierarchical Porous Structure of Engineered Carbon Nanospaces for Use in Hydrogen Storage. MICHAEL KRAUS, JACOB BURRESS, MATTHEW BECKNER, CARLOS WEXLER, PETER PFEIFER, Dept. of Physics and Astronomy, Univ. of Missouri — High-surface-area activated carbons are promising material for hydrogen storage. Mapping the pore structure at the nanometer scale is fundamental for the understanding of adsorptive properties. Structural analyses of pores in nanoporous carbons, using subcritical nitrogen adsorption, supercrITICAL methane adsorption, and small-angle x-ray scattering (SAXS), are presented. Adsorption isotherms provide pore-size distributions, while SAXS provides information about the spatial arrangement of pores. At large length scales, ~20-2000 nm, our samples exhibit an extended regime of surface fractal behavior with a fractal dimension of ~2.3, corresponding to a mild external roughness of the samples. At small length scales, the samples exhibit an abundance of pores 0.5-1.5 nm wide. An illustrative case exhibits cylindrical pores with average width of 0.9 nm and average length 1.6 nm, in excellent agreement with structural data inferred from adsorption isotherms. Comparison of pore data from SAXS and nitrogen isotherms will be compared with hydrogen uptake isotherms. This material is based on work supported by the U.S. Department of Energy under Award No. DE-FG-08GO18142. Use of the Advanced Photon Source was supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.
1:27PM W27.00012 Analysis of Hydrogen Adsorption in Engineered Carbon Nanospaces. JACOB BURRESS, MATTHEW BECKNER, NICK KÜLLMAN, RAINA CEPEL, CARLOS WEXLER, PETER PFEIFER, Dept. of Physics and Astronomy, University of Missouri — We present a survey of how appropriately engineered nanoporous carbons provide materials for reversible hydrogen storage, based on physisorption, with exceptional storage capacities (~80 g H2/kg carbon, ~50 g H2/liter carbon, at 50 bar and 77 K). The H2 gas-carbon surface interface physics was investigated using supercritical hydrogen isotherms. Experimental case studies, with surface areas as high as 3500 m2/g, in which 40% of all surface sites reside in pores of width ~0.7 nm and binding energy ~9 kJ/mol, and 60% of sites in pores of width >1.0 nm and binding energy ~5 kJ/mol, are also presented. We experimentally distinguish between mobile and local adsorption, how lateral dynamics affect the hydrogen storage capacity, and how the two situations are controlled by the vibrational frequencies of adsorbed hydrogen molecules parallel and perpendicular to the surface. In our samples, adsorption is mobile at 293 K, and localized at 77 K. These findings present evidence hydrogen storage capacities in nanoporous carbons can be increased, without any chemical surface functionalization, by more than a factor of two by suitable engineering of the nanopore space. This material is based on work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46411.

1:39PM W27.00013 Quantum energy levels of hydrogen adsorbed on nanoporous carbons: an intrinsic probe for pore structure, and improving Monte Carlo simulations of adsorption1. R. CEPEL, Univ. of Missouri, B. KUCHTA, Univ. de Provence, L. FIRLEJ, Univ. Montpellier 2, RAINA CEPEL, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Carbons are one of potentially promising groups of materials for hydrogen storage by adsorption. However, the heat of hydrogen physisorption in such materials is low, in the range of about 4-8 kJ/mol which limits the total amount of hydrogen adsorbed at P = 100 bar to ~2 wt% at room temperature and about ~10 wt% at all conditions. To get better storage capacity, the adsorbing surfaces must be modified, either by substitution of some atoms in the all-carbon skeleton by other elements, or by doping/intercalation with other species. Here we analyze the variation of interaction energy between a molecule of hydrogen and graphene-based sorbents prepared as hypothetical modifications of the graphene layer. In particular, we show that partial substitution of carbons (for example, by boron) modifies both the symmetry of the energy landscape and strength of hydrogen physisorption. The effect of substituent extends over several sites of graphene lattice making the surface more heterogeneous.

1:51PM W27.00014 Structural and energetic factors in designing a perfect nano-porous sorbent for hydrogen storage1. BOGDAN KUCHTA, Université de Provence, LUCYNA FIRLEJ, Université Montpellier 2, RAINA CEPEL, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Carbons are one of potentially promising groups of materials for hydrogen storage by adsorption. However, the heat of hydrogen physisorption in such materials is low, in the range of about 4-8 kJ/mol which limits the total amount of hydrogen adsorbed at P = 100 bar to ~2 wt% at room temperature and about ~10 wt% at all conditions. To get better storage capacity, the adsorbing surfaces must be modified, either by substitution of some atoms in the all-carbon skeleton by other elements, or by doping/intercalation with other species. Here we analyze the variation of interaction energy between a molecule of hydrogen and graphene-based sorbents prepared as hypothetical modifications of the graphene layer. In particular, we show that partial substitution of carbons (for example, by boron) modifies both the symmetry of the energy landscape and strength of hydrogen physisorption. The effect of substituent extends over several sites of graphene lattice making the surface more heterogeneous.

1 This material is based on work supported by the U.S. Department of Energy under Award No. DE-FG02-07ER46411.

Thursday, March 19, 2009 11:15AM - 2:15PM - Session W28 FIAP DMP: Focus Session: Device Applications of Multiferroic Structures

11:15AM W28.00001 Multiferroic Microwave and Millimeter Wave Devices, GOPALAN SRINIVASAN, Oakland University — Layered composites of ferrites and ferroelectrics are magneto-electric (ME) multiferroics and are of interest for studies on the physics of ME interactions and for novel signal processing devices. There are two types of interactions. (i) ME coupling in bound ferrite-piezoelectrics: An electric field E applied to the composite produces a mechanical deformation in the piezoelectric phase that in turn is coupled to the ferrite, resulting in a shift in the ferromagnetic resonance field. The strength of the interactions is measured from the FMR shifts. (ii) ME interactions in unbound ferrite-ferroelectrics: This is a proximity effect in which hybrid spin-electromagnetic waves are formed. An electric field applied to the ferroelectric will result in a change in the permittivity and a shift in the hybrid modes. We performed studies on the nature of ME interactions at 1-110 GHz in bilayers of epitaxial yttrium iron garnet (YIG) films, single crystal spinel ferrites or hexagonal ferrites and single crystal lead magnesium niobate-lead titanate (PMN-PT) or polycrystalline lead zirconium titanate (PZT). A stripline structure or a cavity resonator was used. Electric fields effects were investigated on magnetostatic waves, uniform precession modes or hybrid modes in the ferrite. We found evidence for strong microwave ME coupling. The coupling strength has been found to be dependent on magnetic field orientation, the nature of piezo-electric coupling and volume for both phases [1]. The high frequency ME effect is of importance for dual electric and magnetic field tunable ferrite-piezoelectric devices. We will discuss the design and characterization of ME resonators, phase shifters, delay lines and filters [2]. The work is supported by grants from the Army Research Office and the office of Naval Research.


11:51AM W28.00002 Electric-field-induced magnetic domain wall motion in bilayer FeGa/BaTiO3 thin film structures1, JOHN CUMINGS, T. BRINTLINGER, S.-H. LIM, Y. QI, L. SALAMANCA-RIBA, I. TAKEUCHI, University of Maryland — We have studied electromechanical coupling induced magnetic domain motion in unclamped FeGa/BaTiO3 thin film bilayer structures. Magnetostriuctive FeGa layers were sputter-deposited on epitaxially grown BaTiO3 films on SrTiO3 substrates. Focused ion-beam milling was used to remove the substrate from underneath the BaTiO3 film, and electrodes were patterned in the metallic FeGa film to apply electric field across a patterned gap (1 micron). Lorentz microscopy was used to monitor the magnetic domains in FeGa, while electric field is applied to the piezoelectric BaTiO3. Lorentz microscopy allows direct and dynamic observation of magnetic domain motions. Reversible electric field induced magnetic domain motion was observed, and the results will be compared to micromagnetic simulations of the domain wall structure.

1 This work is funded by NSF MRSEC (DMR 0520471), ONR-MURI N000140610530 and ARO W911NF-07-1-0410.
12:03PM W28.00003 Ferroelectric control of magnetization in BiFeO3/CoFe heterostructures. MARTIN GAJEK, LANE MARTIN, JOHN HERON, JAN SEIDEL, University of California at Berkeley, CONCEPT GROUP BERKELEY TEAM — The cross coupling between ferroic order parameters in multiferroics opens an alternative for the control of magnetism in magnetoelectric devices by purely electrical means. We first report on the exchange coupling between BiFeO3, an antiferromagnetic ferroelectric, and CoFe. We then show that the domain structure of the ferromagnet can be changed by poling the ferroelectric layer. Finally, we will discuss the implementation of our findings into possible device schemes.

12:15PM W28.00004 Induced magnetization in ferroelectric-antiperovskite heterostructure. PAVEL LUKASHEV, RENAT SABIRIANOV, University of Nebraska, Omaha — We theoretically predict the linear magnetoelectric effect (ME) in ferroelectric-antiperovskite PbTiO3/Mn3GaN heterostructure. The effect is caused by the recently reported piezomagnetic nature of the Mn3GaN. Elastic deformations in the Mn3GaN are due to the surface strain and the soft mode atomic displacements from ferroelectric to the antiperovskite (AP) phase. Both mechanisms lower the symmetry of the AP component, which results in the induced magnetization. Reversal of the polarization direction in the ferroelectric phase results in the magnetization reversal in Mn3GaN, thus the observed effect is linear. We study few interface geometries to account for the electrostatic complementarity at the surface. Those interfaces, which are electrostatically incompatible exhibit strong tetragonal distortion of the cell. The induced magnetization depends on the termination of the components of the heterostructure, and ranges from 0.25 \( \mu_B \) to 0.6 \( \mu_B \) per unit cell of Mn3GaN. All calculations were performed by projector augmented wave method.

12:27PM W28.00005 Magnetoelectric Coupling in Complex Oxide Heterostructures. JASON HOFFMAN, CARLOS VAZ, Department of Applied Physics, Yale University, HAJO MOLEGRAAF, University of Twente, JEAN-MARC TRISCONE, University of Geneva, CHARLES AHN, Department of Applied Physics, Yale University — Current efforts to use materials with multifunctional capabilities have renewed interest in multiferroics, which display a coupling between ferroic order parameters. Engineered structures that combine dissimilar magnetic and ferroelectric systems epitaxially have been shown to exhibit enhanced magnetoelectric coupling. In this work, off-axis RF magnetron sputtering was used to deposit epitaxial ferroelectric Pb(Zr,Ti)O3 (PZT) / La0.6Sr0.4MnO3 (LSMO) heterostructures with high crystalline quality and atomically smooth surfaces. X-ray diffraction shows c-axis oriented growth of PZT, with a typical root-mean-square (RMS) surface roughness of 5Å. We employ magneto-optic Kerr effect (MOKE) magnetometry to study directly the local magnetic state of the LSMO as a function of the PZT polarization state. We demonstrate direct control of magnetism via applied electric fields, including on/off switching of magnetism. The coupling between magnetic and electric order parameters in ferroelectric / Sr-doped lanthanum manganite heterostructures is illustrated by hysteretic M-E (magnetization vs. electric field) loops, with a measured magnetoelastic susceptibility of \( a \sim 10 \text{ cm} / \text{kV}^{-1} \).

12:39PM W28.00006 GaMnAs-based hybrid multiferroic memory device. LEONID ROKHINSON, Purdue University — A rapidly developing field of spintronics is based on the premise that substituting charge with spin as a carrier of information can lead to new devices with lower power consumption, non-volatility and high operational speed. Despite efficient magnetization detection, magnetization manipulation is primarily performed by current-generated local magnetic fields and is very inefficient. Here we report a novel non-volatile hybrid multiferroic memory cell with electrostatic control of magnetization based on strain-coupled GaMnAs ferromagnetic semiconductor and a piezoelectric material. We use the crystalline anisotropy of GaMnAs to store information in the orientation of the magnetization along one of the two easy axes, which is monitored via transverse anisotropic magnetoresistance. The magnetization orientation is switched by applying voltage to the piezoelectric material and tuning magnetic anisotropy of GaMnAs via the resulting stress field.

1:15PM W28.00007 Exchange Coupling across BiFeO3/La0.7Sr0.3MnO3 Interface. PU YU, M. HUIJBEREN, M.B. HOLCOMB, C.H. YANG, Q. HE, Y. H. CHU, J. X. ZHANG, L. W. MARTIN, R. RAMESH, Department of Physics and Department of Materials Science and Engineering, University of California, Berkeley, PER-ANDERS GLANS, J. H. GUO, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley — Controlling the magnetic state by using electric field is a central topic for spintronics and has piqued intense interest. The coupling of antiferromagnetic and ferroelectric order parameters of multiferroic BiFeO3 (BFO) provides a new approach to achieve this goal by using exchange coupling effect. Our previous studies have shown negative exchange bias between epitaxial ferromagnetic La0.6Sr0.4MnO3 (LSMO) and BFO heterostructures and magnetoelectric coupling at these interfaces. The coupling mechanism between these two materials is still a mystery due to the complexity of the G-type spin structure. In this work, by controlling the domain structures of BFO and studying the corresponding exchange coupling effect, the possible coupling mechanism of antiferromagnetic and ferromagnetic spin structures will be proposed. Additionally, the coupling of orbits across the interface will also be discussed, which will give us another possible clue to understand the spin coupling mechanism, since usually orbital and spin orders are coupled together.

1:27PM W28.00008 Electric field tuning of magnetic properties in FeGa films on ferroelastic Pb(Zr,Ti)O3 thin films probed by ferromagnetic resonance. ARUN LUYKX, SAMUEL LOFLAND, VARATHRAJAN ANBUSATHAIAH, VALANOKO NAGARAJAN, FRANISKA KARTAWIDJAJA, JOHN WANG, ICHIRO TAKEUCHI — In order to investigate the possibility of fabricating electric field tunable thin film magnetic devices using a ferroelastic transduction effect, we have patterned Fe80-Ga20 (FeGa) films sputter-deposited on PbZr0.3Ti0.7O3 (PZT(70/30)) / PbZr0.7Ti0.3O3 (PZT(70/30)) tetragonal/rhombohedral bilayers on Pt/Ti/SiO2/Si wafers. Previous piezoferroscopy microscopy studies have shown that the PZT bilayers exhibit presence of ferroelastic domains where the fraction of the local c/a domain ratio can be tuned by an applied electric field. The FeGa top layer was patterned into 20 \( \mu \text{m} \times 20 \mu \text{m} \) capacitor devices in order to apply electric field to the multilayers, and ferromagnetic resonance (FMR) measurements at 9.2 GHz were performed. Typically, a relatively sharp FMR signal observed before application of the electric field would get substantially broadened after initial application of +4 kV/cm. Angular dependent FMR indicates that magnetic anisotropy in the FeGa is indeed affected by application of electric field.

1:39PM W28.00009 Magnetoelectric/piezoelectric laminated structures for tunable remote contact-less magnetic sensing and energy harvesting. PETER FINKEL, Drexel University — We report a method for tunable, contact-less, magnetic field sensing using magnetoelectric coupling properties of the magnetoelectric/piezoelectric laminated composite structure. The magnetically tunable, flexural resonant mode in the bimorph FeNi36% (invar) / PVDF clamped cantilever has been investigated as a function of stress and external magnetic field using Doppler laser spectroscopy. Here we demonstrated that this bimorph structure can be used for low frequency contact-less detection of magnetic field fluctuation and magnetic field monitoring.
suggesting that the magnetic moments for the f-electrons play a significant role. and interband scattering to the Gilbert damping parameter. The Y/Ag/(Fe, Co) trilayers seems not to change the resonance linewidth from the bulk value, for Ag/TM/Ag, while Ni and Py in the trilayer films show equal or larger linewidths. We attribute this behavior to the relative contributions of intraband
magnetic properties of rare earth (Gd, Tb, Sm)/Ag/transition metal (Fe, Co, Ni and Py) trilayers by ferromagnetic resonance technique. We found that Fe
of Texas at Arlington, MYRON B. SALAMON, Department of Physics, University of Texas at Dallas — We have investigated temperature dependent dynamic
FMR linewidths
1
configurations by spin-polarized current.
Simulations show that these unusual features of spin torque dynamics are due to the second-order perpendicular magnetic anisotropy term at the Co/Pt
states. In the regime of current-driven persistent magnetization precession, we observe unusual non-monotonic dependence of the precession frequency on
current. However, we are currently not able to explain the asymmetry in the precession frequency observed for Ni/Pt. The dynamical coupling between
ferromagnets due to ST can induce dynamical states in magnetic multilayer nanopillars not accessible by any other techniques. For in-plane magnetic field, the predicted dynamical
regimes include elliptical, clamshell, and out-of-plane precession. The first two regimes have been demonstrated and extensively analyzed. However, the
out-of-plane precession has so far been elusive. Calculations [1] show that dynamical coupling between ferromagnets due to ST can result in suppression of
precession for one of the current polarities. We interpret our results in terms of the dynamical coupling between magnetic layers due to spin transfer, completely
suppressing precession of the thicker layer.

Thursday, March 19, 2009 11:15AM - 2:15PM –
Session W29 GMAG DMP FIAP: Focus Session: Current-Induced Oscillations 333

11:15AM W29.00001 Competition between orbital torques and spin polarization in controlling
FMRI linewidths
1
SEZEN DEMIRTAŞ, Department of Physics, University of Texas at Dallas, ALI R. KOYMEN, Department of Physics, University of Texas at Arlington, MYRON B. SALAMON, Department of Physics, University of Texas at Dallas — We have investigated temperature dependent dynamic
magnetic properties of rare earth (Gd, Tb, Sm)/Ag/transition metal (Fe, Co, Ni and Py) trilayers by ferromagnetic resonance technique. We found that Fe
and Co among TM (transition metals) show narrower magnetic resonance linewidths in rare earth (RE)/Ag/RE/Ag thin film trilayers compared to the values for Ag/Ag/Ag, while Ni and Pd in the trilayer films show equal or larger linewidths. We attribute this behavior to the relative contributions of intraband and interband scattering to the Gilbert damping parameter. The Y/Ag/(Fe, Co) trilayers seems not to change the resonance linewidth from the bulk value, suggesting that the magnetic moments for the f-electrons play a significant role.

11:27AM W29.00002 Current-induced dynamics in almost symmetric magnetic nanopillars
1
SERGEI URAZHDIN, WENG LIM, ANDREW HIGGINS, West Virginia University — Magnetic nanodevices usually include a free layer whose configuration can
be changed by spin-polarized current via the spin transfer (ST), and a fixed reference (polarizing) layer. The polarizer is usually made much larger than the
free layer to minimize the effects of ST. However, it is presently not known what makes a specific magnetic layer behave as a fixed polarizer or a free layer
driven by ST. Little is also known about the dynamics in bilayers with thin polarizers, where the effects of ST on both layers are significant. We will discuss our
spectroscopic measurements of current-induced dynamics in nanopillars with similar thicknesses of the extended polarizer and the nanopatterned free layer. We
demonstrate coherent out-of-plane precession for both polarities of current in symmetric devices. However, even slightly asymmetric devices exhibit a rapid suppression of
precession for one of the current polarities. We interpret our results in terms of the dynamical coupling between magnetic layers due to spin transfer, completely
suppressing precession of the thicker layer.

1Supported by NSF DMR-0747609 and a Cottrell Scholarship from Research Corporation.

11:39AM W29.00003 Measurements of out-of-plane dynamics induced by spin transfer in magnetic
nanopillars
1
WENG LIM, West Virginia University, SERGEI URAZHDIN, West Virginia University — Current-induced spin transfer (ST) can induce dynamic states in magnetic multilayer nanopillars not accessible by any other techniques. For in-plane magnetic field, the predicted dynamical
regimes include elliptical, clamshell, and out-of-plane precession. The first two regimes have been demonstrated and extensively analyzed. However, the
out-of-plane precession has so far been elusive. Calculations [1] show that dynamical coupling between ferromagnets due to ST can result in suppression of
coherent out-of-plane precession in nanopillars with a patterned polarizing layer, which is the geometry studied so far. We will discuss our measurements of current-induced dynamics in nanopillars with extended polarizer, in which the decoherence caused by the coupling between magnetic layers is minimized. We
demonstrate coherent out-of-plane precession, whose dependence on current and the direction of the magnetic field is consistent with micromagnetic simulations. Most surprisingly, our data are asymmetric with respect to reversal of the magnetic field, which is explained by a combination of the Oersted field and sample shape imperfections. [1] S. Urazhdin, Phys. Rev. B 78, 060405(R) (2008).

1Supported by NSF DMR-0747609 and a Cottrell Scholarship from Research Corporation.

11:51AM W29.00004 Spin Torque Dynamics of Nanomagnets with Weak Magnetic Anisotropy
HOANG YEN T. NGUYEN, XIAO CHENG, CARL BOONE, JIAN ZHU, ILYA KRIVOKROTTOV, Department of Physics and Astronomy, University of California, Irvine — We study switching and persistent precession of magnetization induced by spin transfer torque in Co(4 nm)/Cu(6 nm)/Co(0.7 nm)/Pt nanopillar spin
valves where perpendicular magnetic anisotropy at the Co/Pt interface nearly cancels the easy-plane shape anisotropy of the free Co layer. We find that in this
system with weak total magnetic anisotropy, spin torque can switch magnetization of the free layer between the in-plane and the out-of-plane static magnetic
states. In the regime of current-driven persistent magnetization precession, we observe unusual non-monotonic dependence of the precession frequency on
current. Simulations show that these unusual features of spin torque dynamics are due to the second-order perpendicular magnetic anisotropy term at the Co/Pt
interface. Our work demonstrates a method for controllable switching of magnetization of a nanomagnet between stable in-plane and out-of-plane magnetic
configurations by spin-polarized current.
12:03PM W29.00005 Slonczewski windmill with dissipation and asymmetry, YAROSLAW BAZALY, University of South Carolina — J. Slonczewski invented spin-transfer effect in layered systems in 1996. Among his first predictions was the regime of the "windmill motion" of a perfectly symmetric spin valve. In this regime magnetizations of the layers rotate in a fixed plane keeping the angle between them constant. Since "windmill" was predicted to happen in the case of zero magnetic anisotropy, while in most experimental setups the anisotropy is significant, the phenomenon was not a subject of much research. However, the behavior of the magnetically isotropic device is related to the interesting question of current-driven transitions between different exchange interaction, and layer asymmetry. It is shown that the windmill rotation is almost always destroyed by those effects, except for a narrow interval of electric current, determined by the parameters of the device.

12:15PM W29.00006 Spin-dependent tunneling effects in magnetic tunnel junctions, LI GAO, IBM Almaden Research Center — It has long been known that current extracted from magnetic electrodes through ultra thin oxide tunnel barriers is spin polarized. This current gives rise to two important properties: tunneling magnetoresistance (TMR) when the tunnel barrier is sandwiched between two thin magnetic electrodes and, spin momentum transfer, which can manipulate the magnetic state of the magnetic electrodes. In the first part of my talk I show how the structure of thin CoFe layers can be made amorphous by simply sandwiching them between two amorphous layers, one of them the tunnel barrier. No glass forming elements are needed. By slightly changing the thickness of these layers or by heating them above their glass transition temperature they become crystalline. Surprisingly, the TMR of the amorphous structure is significantly higher than of its crystalline counterpart. The tunneling anisotropic magnetoresistance, which has complex voltage dependence, is also discussed. In the second part of my talk I discuss the microwave emission spectrum from magnetic tunnel junctions induced by spin torque from spin polarized dc current passed through the device. We show that the spectrum is very sensitive to small variations in device structures, even in those devices which exhibit similarly high TMR (~120%) and which have similar resistance-area products (~4-10 Ωm²). We speculate that these variations are due to non-uniform spatial magnetic excitation arising from inhomogeneous current flow through the tunnel barrier. [In collaboration with Xing Jiang, M. Hayashi, Rai Moriya, Brian Hughes, Teya Topuria, Phil Rice, and Stuart S.P. Parkin]

12:15PM W29.00007 Frequency-doubling spin-torque microwave oscillator, GRAHAM ROWLANDS, ILYA KRIVOROTOV, University of California, Irvine — We describe a new type of spin torque oscillator with two free layers that is capable of emitting high microwave power (> 1 mW) at high frequency (> 50 GHz) in zero external field. This device has two perpendicular-anisotropy fixed ferromagnetic layers and two easy-plane free layers sandwiched between the fixed layers, with all of the magnetic layers separated from each other by non-magnetic spacers. We simulate current-driven magnetization dynamics in this structure in the macrospin approximation, taking into account spin-torque interactions between adjacent ferromagnetic layers. Our simulations show that for both fixed layers magnetized in the same direction perpendicular to the plane of the sample, spin-torque induces clockwise rotation of one of the layers and counterclockwise rotation of the other. This type of current-driven dynamics gives rise to large-amplitude microwave signal with the frequency that is the sum of the precession frequencies of the free layers. We study the effect of dipolar coupling, shape anisotropy and external field on the dynamics of this spin torque oscillator and determine the optimal device parameters for high-amplitude high-frequency microwave signal generation.

1:03PM W29.00008 Spectral Line Shape and Line Width of a Single-Mode Spin Torque Oscillator, ILYA KRIVOROTOV, CARL BOONE, JIAN ZHU, XIAO CHENG, Department of Physics and Astronomy, University of California, Irvine, JORDAN KATINE, JEFF CHILDRESS, Hitachi Global Storage Technologies — Spin torque auto-oscillators are strongly nonlinear dynamical systems that are highly susceptible to external perturbations such as spin-polarized current and temperature. To understand the effect of thermal fluctuations on the oscillator dynamics, we measure power spectrum of single-mode spin torque oscillators based on a GMR nanocontact to a permalloy nanowire. Our measurements reveal deviations of the power spectral line shape from a simple Lorentzian. These deviations can be understood in terms of dephasing induced by the oscillator amplitude fluctuations. The measured spectral line shape is in a good agreement with a recent analytic theory of spin torque oscillator dynamics at a non-zero temperature [1]. We show that precise measurements of the line shape give information on important oscillator parameters such as Gilbert damping in the large-amplitude regime of current-driven magnetization dynamics. [1] V. S. Tiberkevich, A. N. Slavin, J.-V. Kim, Phys. Rev. B 78, 092401 (2008).

1:15PM W29.00009 Time domain studies of aperiodicity in spin-torque driven vortex oscillations, VLAD PRIBIAG, B. WILLIAMS, A. STEHURA, D.C. RALPH, R.A. BUHRMAN, Cornell University, CORNELL TEAM — Previous studies of current-driven magnetic vortex oscillations in nanopillars [1] and point contact geometries [2] have been restricted to detection of the average envelope of the oscillations. In this talk we discuss aperiodic features of the vortex oscillations that were studied using single-shot time domain measurements of the oscillating GMR signal. These measurements reveal stochastic mode jumping at 10's of ms mean duty cycles between several closely spaced frequencies. The power spectrum of the time traces indicates that the shape and amplitude of the oscillation’s spectral peaks change abruptly as the function of time, corresponding to aperiodic modulation of these oscillations on the µs time scale. Due to the very narrow long-time linewidths of the oscillations it is possible to detect clearly these fine modulations of the peak shape, frequency and amplitude. From these studies of the spin-torque-driven vortex oscillator stability we seek to obtain insights for the design and fabrication of spin-torque oscillators with even narrower linewidths. [1] V.S. Pribiag et al., Nature Phys. 3, 498 (2007). [2] Q. Mistral et al., Phys. Rev. Lett. 100, 257201 (2008).

1:27PM W29.00010 The Role of Spin-Motive Forces in Spin-Valve Dynamics, JUN’ICHI IEDA, SADAMICHI MAEKAWA, Tohoku University; CREST-JST, STEWART E. BARNES, University of Miami — A spin-motive force (smf) is the counterpart of an electro-motive force, which couples to the spin rather than charge degrees of freedom of electrons. Here we discuss how smfs work in spin-valves. When the magnetization makes a sudden change, there often appears a large peak in dV/dl, i.e., a voltage jump that is better interpreted in terms of smfs. To see this, we model spin-valves using an equivalent circuit that involves magnetic dissipation represented by smfs as well as electric dissipation through ordinary resistors for both majority and minority currents. There are four possible conduction paths, e.g., the majority electrons hop to the majority band, or to the minority band and vice versa. The first path adds an up electron to the free layer and causes a rotation in a certain sense, while the second path adds a down electron and a rotation in the opposite sense. Since the rotations are in opposite senses so is the work done on the free layer and hence the smf. By solving the circuit problem and the Landau-Lifshitz equations supplemented with the Slonczewski torque-transfer term simultaneously we find the spin-transfer effect is dramatically modified by smfs. With the relevant parameters a stable large angle precession and a voltage signal are predicted.

1:39PM W29.00011 Mutual phase-locking and frustration of interaction in arrays of interacting spin-torque nano-oscillators, ANDREI SLAVIN, VASIL TIBERKEVICH, Oakland University — We developed a perturbation theory describing collective dynamics of spin-torque nano-oscillator (STNO) arrays in a weak-coupling limit. In this limit each STNO is described by a single dynamical variable – effective phase φj, which satisfies the equation dφj/dt = ωj + ∑k λjk sin(φj - φk + βjk). Here ωj is the free-running (unperturbed) frequency of the j-th oscillator, λjk is the effective coupling amplitude of j-th and k-th oscillators, and βjk is the frustration angle of the oscillators’ interactions. The frustration angles βjk are determined by the intrinsic nonlinearities of STNO and by the delay of coupling signals. The frustration angles can be controlled by changing the distance between STNOs and/or by adding reactive elements to the STNO circuit. We have analyzed collective dynamics of STNO arrays in the case of global coupling, i.e. when coupling amplitudes and frustration angles for all STNOs are equal, λjk = λ, βjk = β. We have shown that STNO array mutually phase-locks only when cos(β) > 0. The critical coupling amplitude λc, at which phase-locking starts, has a minimum for cos(β) = 1 (i.e., for β = 2π), and increases with the decrease of cos(β). For cos(β) < 0 the mutual phase-locking of more than two STNOs is impossible, and the STNO array enters a frustrated state, in which the output power becomes vanishingly small due to the destructive interference between individual STNOs.

1:39PM W29.00012 Mutual phase-locking and frustration of interaction in arrays of interacting spin-torque nano-oscillators, ANDREI SLAVIN, VASIL TIBERKEVICH, Oakland University — We developed a perturbation theory describing collective dynamics of spin-torque nano-oscillator (STNO) arrays in a weak-coupling limit. In this limit each STNO is described by a single dynamical variable – effective phase φj, which satisfies the equation dφj/dt = ωj + ∑k λjk sin(φj - φk + βjk). Here ωj is the free-running (unperturbed) frequency of the j-th oscillator, λjk is the effective coupling amplitude of j-th and k-th oscillators, and βjk is the frustration angle of the oscillators’ interactions. The frustration angles βjk are determined by the intrinsic nonlinearities of STNO and by the delay of coupling signals. The frustration angles can be controlled by changing the distance between STNOs and/or by adding reactive elements to the STNO circuit. We have analyzed collective dynamics of STNO arrays in the case of global coupling, i.e. when coupling amplitudes and frustration angles for all STNOs are equal, λjk = λ, βjk = β. We have shown that STNO array mutually phase-locks only when cos(β) > 0. The critical coupling amplitude λc, at which phase-locking starts, has a minimum for cos(β) = 1 (i.e., for β = 2π), and increases with the decrease of cos(β). For cos(β) < 0 the mutual phase-locking of more than two STNOs is impossible, and the STNO array enters a frustrated state, in which the output power becomes vanishingly small due to the destructive interference between individual STNOs.
1:51PM W29.00012 Spin-torque-driven ferromagnetic resonance in a nonlinear regime\textsuperscript{1}, WENYU CHEN\textsuperscript{2}, G. DE LOUBENS\textsuperscript{3}, J.-M. L. BEAUJOUR, Dept. of Physics, NYU, J. Z. SUN, IBM T. J. Watson Research Center, A. D. KENT, Dept. of Physics, NYU — Spin-torque-driven ferromagnetic resonance (ST-FMR) is a quantitative tool for studying spin-transfer interactions in nanojunctions. Using this method we have studied Co/Cu/CoNi spin valves, in which the CoNi synthetic free layer has perpendicular magnetic anisotropy. Perpendicular field swept resonance lines were measured under a large amplitude GHz current excitation, which drove ST-FMR into a nonlinear regime and produced a large angle precession of the free layer magnetization. With increasing rf power, the resonance lines deviate from a Lorentzian shape and became asymmetric, with a lower resonance field and a larger linewidth. A non-hysteretic step jump in ST-FMR voltage signal was also observed at high powers. The comparison of the experimental results to the foldover and the nonlinear damping theories will be presented.

\textsuperscript{1}This research was supported by NSF-DMR-0706322.
\textsuperscript{2}Currently at Hitachi Global Storage Technologies, San Jose, CA 95135
\textsuperscript{3}present address: SPEC, CEA Saclay, France

2:03PM W29.00013 Microwave oscillation generation in a Co/Cu/Co nano-contact without external magnetic field\textsuperscript{1}, KWUN HUNG CHEUNG, XIN XIAO, HONG WEN JIANG, UCLA Physics Department — Using spin-transfer-torque effect to generate microwave oscillation at zero magnetic-field is of recent interest. Here, we report the observation a resistive oscillation at microwave-frequencies ranging from 1.5 to 3 GHz in a nano-contact formed on a Co/Cu/Co tri-layer structure without any external field. The observed oscillation modes have frequencies that are much higher than that reported in other similar experimental systems [1,2]. We have studied the evolution of the oscillation as a function of the DC excitation current and the effect of a small in-plane field. Micromagnetic simulations support the notion that the oscillation is a result of the translational motion of a vortex-core underneath the nano-contact, due the competition of the circular Orstead field and the spin-transfer torque, both induced by the DC current passing through the nano-contact. The work was supported by the Western Institute of Nanoelectronics (WIN). [1] M. R. Pufall et al., Phys. Rev. B 75, 140404(R) (2007). [2] Q. Mishra et al., Phys. Rev Lett. 100, 257201 (2008).

\textsuperscript{1}The work was supported by the Western Institute of Nanoelectronics (WIN).

Thursday, March 19, 2009 11:15AM - 2:15PM –
Session W30 DMP GMAG: Focus Session: Ruthenates 334

11:15AM W30.00001 Ca\textsubscript{3}(Ru\textsubscript{1-x}Cr\textsubscript{x})\textsubscript{2}O\textsubscript{7}: A new paradigm for spin valves\textsuperscript{1}, GANG CAO, University of Kentucky — A spin valve is a device structure whose electrical resistance can be manipulated by controlling the relative spin alignment of adjacent metallic, magnetic layers separated by nonmagnetic insulating layers. The spin valve effect is a quantum phenomenon so far only realized in multilayer thin films or bulk.

\textsuperscript{1}In collaboration with V. Durairaj, S. Chikara, Dr. L. DeLong and Dr. P. Schlottmann. This work was supported by NSF through grant DMR-0552267

11:51AM W30.00002 Antiferromagnetism and bulk spin valve effect in Ca\textsubscript{3}(Ru\textsubscript{1-x}Ti\textsubscript{x})\textsubscript{2}O\textsubscript{7}. J. PENG, T.J. LIU, Z. QU, E. VEHSTEDT, B. QIAN, D. FOBES, Tulane University, L. SPINU, University of New Orleans, W. BAO, Los Alamos National Laboratory, Z.Q. MAO, Tulane University — Ca\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} has generated growing interest. It shows an antiferromagnetic (AFM) transition at \(T_N = 56\) K, followed by a metal-insulator (MI) transition at \(T_{M1} = 48\) K [1]. Giant magnetoresistance (GMR) across its metamagnetic transition is also observed. We have determined the magnetic structures of Ca\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} under magnetic fields using neutron scattering [2]. Our results demonstrate that the GMR in this material originates from a bulk spin-valve effect, and clarifies the origin for the puzzling observation that the GMR occurs under easy axis field alignment, while a colossal magnetoresistance appears with hard axis field alignment [1].


12:03PM W30.00003 Antiferromagnetic Metallic State And Spin Valve Effect in Doped (Ca\textsubscript{1-x}A\textsubscript{x})\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} (A = Sr, Ba) Single Crystals\textsuperscript{1}, S. CHIKARA, O.B. KORNETA, T.F. QI, S. PARKIN, G. CAO, Univ. of Kentucky, W.P. SONG, Inst. of Solid State Physics, Hefei 230031, P.R. China, W.P. CRUMMETT, Centre College, KY40422 — Bilayered Ca\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} is a highly anisotropic system [1] characterized by orbitally-driven colossal magnetoresistance\textsuperscript{2} and an unusual antiferromagnetic metallic (AFM-M) state [2]. We report transport and thermodynamic properties of (Ca\textsubscript{1-x}A\textsubscript{x})\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} (A = Sr, Ba) single crystals as a function of temperature and applied magnetic field. While Ba doping shows a far stronger impact, both Sr and Ba substitution for Ca induce a large array of interesting phenomena. Among them, a bulk spin-valve effect occurs in the AFM-M range, which is largely broadened due to the doping. This effect in bulk crystals is a novel phenomenon first observed in Ca\textsubscript{3}(Ru\textsubscript{1-x}Cr\textsubscript{x})\textsubscript{2}O\textsubscript{7} single crystals [3]. The spin-valve effect in (Ca\textsubscript{1-x}A\textsubscript{x})\textsubscript{3}Ru\textsubscript{2}O\textsubscript{7} single crystals opens new avenues to understand the underlying physics and realize the potential of spin valves in practical devices.


\textsuperscript{1}This work was supported by NSF through grant DMR-0552267.
However, there are little changes of the core-level satellite features with \( n \), suggesting the electron-electron correlation is mainly confined in the RuO\(_3\) Sr\(_2\) perovskite crystal \( \text{Sr} \). LIU, DAVID FOBES, ZHIQIANG MAO, Physics Department, Tulane University, New Orleans, LA 70118, USA — Core-level photoelectron spectra of the layered

Tokyo, Y. YOSHIDA, National Institute of Advanced Industrial Science and Technology (AIST), A. TANAKA, Hiroshima University, I.S. ELFIMOV, G.A. BERRIDGE, ANDREW GREEN, SANTIAGO GRIGERA, University of St Andrews, BEN SIMONS, University of Cambridge — The phase diagram of \( \text{SrRuO}_3 \)

contains a metamagnetic transition that bifurcates to enclose an anomalous phase with intriguing properties - a large resistivity with anisotropy that breaks the magnetic scattering, for the nearly FM region

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magnetic properties. The magnetic ground state ranges from an itinerant metamagnetic state

\( x < \), and finally to an antiferromagnetic (AFM) state

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et al. [1]. For nearly degenerate bands, spin-orbit coupling leads to a dramatic change of the Fermi surface warping. Above the transition field, under polar rotation we observe a first order phase transition in \( \rho_{xy} \) for angles close to the ab-plane clearly indicating a polarization of the \( 4d_{xy,yz} \) orbitals. Additionally, we have performed similar studies on \( \text{Sr}_{2-x} \text{Ru}_{2} \text{O}_{6} \), and have observed preliminary evidence of orbital-dependent magnetic correlations. This work is supported by the NSF under grant DMR-0645305, the DOE under DE-FG02-07ER46358.


12:39PM W30.00006 Electronic phase diagram in double layered ruthenates (\( \text{Sr}_{1-x}\text{Ca}_x\text{Ru}_2\text{O}_7 \)), Z.Q. MAO, Z. QU, PENG, T.J. LIU, D. FOBES, B. QIAN, Tulane University, L. SPINU, University of New Orleans — We previously established a magnetic phase diagram for (\( \text{Sr}_{1-x}\text{Ca}_x\text{Ru}_2\text{O}_7 \)) (0 \( x \leq 1 \)) using high quality single crystals grown by a floating-zone method [1]. This phase diagram exhibits rich magnetic properties. The magnetic ground state ranges from an itinerant metamagnetic state (0 \( x < 0.08 \)), to an unusual heavy-mass, nearly ferromagnetic (FM) state (0.08 \( x < 0.4 \)), and finally to an antiferromagnetic (AFM) state (0.4 \( x < 1 \)). In this talk we report the electronic properties of these magnetic states. We will show that the electronic and magnetic properties are strongly coupled in this system. The electronic ground state evolves from an AFM quasi-two-dimensional metal for \( x = 1.0 \), to an Anderson localized state for the AFM region 0.4 \( x < 1.0 \), and then to a weakly localized state, induced by magnetic scattering, for the nearly FM region 0.08 \( x < 0.4 \). When \( x \) approaches the critical composition 0.08, the localization weakens and non-Fermi liquid (FL) behavior occurs. The system eventually transforms into a FL ground state when the magnetic ground state switches to the itinerant metamagnetic state for \( x < 0.08 \). These results demonstrate the delicate balance among the charge, spin, lattice and orbital degrees of freedom in ruthenates.


12:51PM W30.00007 Inhomogeneous magnetic phases: a LOFF-like phase in \( \text{Sr}_2\text{Ru}_2\text{O}_7 \), ANDREW BERRIDGE, ANDREW GREEN, SANTIAGO GRIGERA, University of St Andrews, BEN SIMONS, University of Cambridge — The phase diagram of \( \text{SrRuO}_3 \) contains a metamagnetic transition that bifurcates to enclose an anomalous phase with intriguing properties - a large resistivity with anisotropy that breaks the crystal-lattice symmetry. We propose that this is a magnetic analogue of the spatially inhomogeneous superconducting Fulde-Ferrel-Larkin-Ovchinnikov state. We show - through a Ginsburg- Landau expansion where the magnetisation transverse to the applied field can become spatially inhomogeneous - that a Stoner model with electronic band dispersion can reproduce this phase diagram and transport behaviour.

1:03PM W30.00008 Crystal-Field Level Inversion in Lightly Mn-Doped \( \text{Sr}_2\text{Ru}_2\text{O}_7 \), MUHAMMED HOSSAIN, University of British Columbia (UBC), Z. HU, M.W. HAVERKORT, T. BURNUS, C.F. CHANG, S. KLEIN, Universität zu Köln, J.D. DENLINGER, Advanced Light Source, LBNL, H.-L. LIN, C.T. CHEN, NSPRC, Taiwan, B. MATTHEI, Y. KANEKO, Y. T. OKURA, S. SATOW, H. TAKAGI, University of Tokyo, Y. YOSHIDA, National Institute of Advanced Industrial Science and Technology (AIST), A. TANAKA, Hiroshima University, I.S. ELFIMOV, G.A. SAWATZKY, UBC, L.H. TENG, Universität zu Köln, A. DAMASCHELLI, UBC — \( \text{Sr}_2(\text{Ru}_{1-x}\text{Mn}_x)\text{O}_3 \), in which 4d-Ru is substituted by the more localized 3d-Mn, is studied by x-ray dichroism and spin-resolved density functional theory. We find that Mn impurities do not exhibit the same +4 valence of Ru, but act as +3 acceptors; the extra e\(_g\) electron occupies the in-plane 3d\(_{2z^2−r^2}\) orbital instead of the expected out-of-plane 3d\(_{xz, yz}\). We propose that the 3d-4d interplay, via the ligand oxygen orbitals, is responsible for this crystal-field level inversion and the material’s transition to an antiferromagnetic, possibly orbitally ordered, low-temperature state. Published: Phys. Rev. Lett. 101, 016404 (2008).

1:15PM W30.00009 Strong spin-orbit coupling effects on the Fermi surface of \( \text{Sr}_2\text{Ru}_2\text{O}_4 \) and \( \text{Sr}_2\text{Rh}_{0.4}\text{Ru}_{0.6} \), ANDREA DAMASCHELLI, University of British Columbia, MAURITS HAVERKORT, MPI Stuttgart, ILYA ELFIMOV, University of British Columbia, HAO TENG, University of Cologne, GEORGE SAWATZKY, University of British Columbia — We present a first-principle study of spin-orbit coupling effects on the Fermi surface of \( \text{Sr}_2\text{Ru}_2\text{O}_4 \) and \( \text{Sr}_2\text{Rh}_{0.4}\text{Ru}_{0.6} \) [1]. For nearly degenerate bands, spin-orbit coupling leads to a dramatic change of the Fermi surface with respect to non-relativistic calculations; as evidenced by the comparison with experiments on \( \text{Sr}_2\text{RhO}_4 \), it cannot be disregarded. For \( \text{Sr}_2\text{Ru}_2\text{O}_4 \), the Fermi surface modifications are so small that they are only barely observable in the material’s transition to an antiferromagnetic, possibly orbitally ordered, low-temperature state. Published: Phys. Rev. Lett. 101, 026406 (2008).

1:27PM W30.00010 Dimensionality and doping effect on the Core-level X-ray photoemission satellites in layered ruthenates,1 HAIZHONG GUO, YI LI, BIAO HU, RONGYING JIN, E.W. PLUMMER, JIANDI ZHANG, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, D. URBINA, Department of Physics, FIU, Miami, FL 33199, USA, TIJJANG LIU, DAVID FOBES, ZHIQIANG MAO, Physics Department, Tulane University, New Orleans, LA 70118, USA — Core-level photoelectron spectra of the layered perovskite crystal \( \text{Sr}_{1+x}\text{Ru}_2\text{O}_{4+x/n} \) (\( n = 1, 2, \) and 3) and Mn-doped \( \text{Sr}_2\text{Ru}_2\text{O}_4 \) are investigated by x-ray photoemission spectroscopy (XPS) techniques. The 3d and Ru 3d core-level spectra exhibit a two-peak structure, screened and unscreened peaks, indicating strong correlation effects among Ru 4d electrons. However, there are little changes of the core-level satellite features with \( n \), suggesting the electron-electron correlation is mainly confined in the RuO\(_2\) plane. On the other hand, doping of Mn will drastically affect the core-level spectral weight, reflecting the doping-induced metal-to-insulator transition in the doped system. The position of Ru-core levels remain the same, thus, indicating no doping-induced change of Ru valence.

[1] The work was supported by NSF-DMR0346826 and DOD AMO-W911NF-07-0532.
1:39PM W30.00011 Magnetic Ordering in Ba$_2$DyRuO$_6^{1}$, J. LAMSAL, Missouri University, W. YELON, Missouri University of Science and Technology. H. BLACKSTEAD, M. SMYLIE, University of Notre Dame, Q. CAI, Missouri University, W. JAMES, J. YANG, Missouri University of Science and Technology — Magnetization measurements and neutron diffraction (ND) studies have been carried out on the double perovskite rhenate, Ba$_2$DyRuO$_6$. The low field magnetization data indicate ordering around 50K, a sharp rise below 8K and a possible transition around 25K. Rietveld analysis of ND data confirms antiferromagnetic ordering at 48K. The temperature dependence of the Ru moment appears to follow a Brillouin type curve down to the lowest temperature accessible, (12K), and there is no evidence for a transition around 25K. In contrast, the Dy moment is found to be proportional to the square of the Ru moment, implying that the Ru moment is the primary order parameter and that Dy ordering is driven by the Ru-Dy coupling. The ND experiment could not reach the temperature at which the magnetization rises sharply (8K), but following similar arguments, we suggest that this point corresponds to the lowest temperature accessible, (12K), and there is no evidence for a transition around 25K. In contrast, the Dy moment is found to be proportional to the square of the Ru moment, implying that the Ru moment is the primary order parameter and that Dy ordering is driven by the Ru-Dy coupling. The ND experiment could not reach the temperature at which the magnetization rises sharply (8K), but following similar arguments, we suggest that this point corresponds to the lowest temperature accessible, (12K), and there is no evidence for a transition around 25K. In contrast, the Dy moment is found to be proportional to the square of the Ru moment, implying that the Ru moment is the primary order parameter and that Dy ordering is driven by the Ru-Dy coupling.

1This work was supported by the NSF.

1:51PM W30.00012 Resistance noise in the bad metal SrRuO$_3^{1}$, FRANCOISE KIDWINGIRA, MICHAEL ROZLER, GERTJAN KOSTER, WOLTER SIEMONS, RIK GROENEN, MALCOLM BEASLEY, Geballe Laboratory for Advanced Materials, Stanford University — SrRuO$_3$ (SRO) is a strongly correlated electrons material with some interesting properties. It is an itinerant ferromagnet below 150K and it transitions from a bad metal at high temperature to a Fermi Liquid at low temperature. In SRO thin films, there is evidence that even a slight presence of Ru deficiencies increases the degree of electron correlations [1]. Using Scanning Tunneling Potentiometry [2], we have studied the local transport properties of this material. The measured resistance has a noise level well above Johnson noise that depends both on the method of synthesis and on the voltage across the sample. We will attempt to characterize these resistance fluctuations with respect to the various unusual properties of the material. [1] W. Siemons et. al., Phys. Rev. B 76, 075126 (2007) [2] M. Rozler and M. R. Beasley, Rev. Sci. Inst 79, 073904 (2008)

1Work supported by BES-DoE.

2:03PM W30.00013 Nyquist noise as probe of hot-electron effects in the ferromagnetic insulating state of manganites$^1$, SUDESHNA SAMANTA, ARUP K. RAYCHAUDHURI, S. N. Bose Centre, Block-JD, Sector-3, Salt-Lake, Kolkata-98, India — Hole-doped rare-earth manganites (like La$_{1-x}$Ca$_x$MnO$_3$) in the ferromagnetic insulating (FMI) state show large non-linear conductance. Such non-linear conductance can arise due to hot-electron effect which originates from decoupling of the electron and lattice temperatures at high power level. The non-linear conductance manifests as electro-resistivity or current induced resistance change. We report here low frequency temperature dependent noise measurement which allows us to estimate the electronic temperature by measuring Nyquist noise in contrast to 1/f noise in La$_{2-x}$Ca$_x$MnO$_3$ single crystals which has a distinct FMI state below 100K. The measurement was performed with low ac biasing current which was mixed with a high current density that leads to electron heating. We observed that in the insulating state, above a certain input d.c power, the Nyquist noise increases by a large extent and this is coupled to the onset of non-linear conduction as signalled by the power dependence of the differential conductance. The experiment establishes a direct link between hot-electron effect and non-linear conductance.

$^1$Financial support from Department of Science and Technology, Govt. of India is acknowledged.

Thursday, March 19, 2009 11:15AM - 2:15PM — Session W31 DMP GMAG: Focus Session: Magnetic Nanoparticles and Nanowires 335

11:15AM W31.00001 Comparative studies of Co nanowires of different diameters electroplated into porous aluminum oxide membranes, ZUXIN YE, HAIDONG LIU, ZHIPING LUO, HAN-GIL LEE, WENHAO WU, D. G. NAUGLE, I. LYUKSYUTOV, Texas A & M University — The correlation between the structural and magnetic properties of template-electroplated Co nanowires has been investigated. Co nanowires of diameters either 65 or 200 nm were fabricated by electroplating Co into the pores of anodic aluminum oxide membranes. Strikingly different structures were observed in these two types of Co nanowires. The 65 nm-thick Co nanowires are composed of long Co single crystal segments with a hexagonal close-packed major phase, while the 200 nm-thick Co nanowires are composed of hexagonal close-packed and face center cubic Co single crystal segments. Correspondingly, different magnetic properties were revealed in these two types of Co nanowires. The 65 nm-thick Co nanowires have a magnetic hysteresis that is significantly larger than that of the 200 nm-thick Co nanowires. In contrast, the 200 nm-thick Co nanowires have large non-linear conductance which results from decoupling of the electron and lattice temperatures at high power level. The non-linear conductance manifests as electro-resistivity or current induced resistance change. We report here low frequency temperature dependent noise measurement which allows us to estimate the electronic temperature by measuring Nyquist noise in contrast to 1/f noise in La$_{2-x}$Ca$_x$MnO$_3$ single crystals which has a distinct FMI state below 100K. The measurement was performed with low ac biasing current which was mixed with a high current density that leads to electron heating. We observed that in the insulating state, above a certain input d.c power, the Nyquist noise increases by a large extent and this is coupled to the onset of non-linear conduction as signalled by the power dependence of the differential conductance. The experiment establishes a direct link between hot-electron effect and non-linear conductance.

11:27AM W31.00002 Self-Assembled Superparamagnetic Binary Nanoparticle Superlattices$^1$, J. CHEN, Dept Mat Sci & Engn, Univ Penn, X. YE, Dept Chem, Univ Penn, Y. ZHANG, Dept Mat Sci & Engn, Univ Penn, J.M. KIKKAWA, Dept Phys & Astron, Univ Penn, C.B. MURRAY, Dept Mat Sci & Engn, Dept Chem, Univ Penn — We report binary nanoparticle superlattices (BNSLs) composed of two different types of superparamagnetic nanoparticles (NPs). Since the magnetic properties of these NPs depend both on size and composition, two strategies are used to form BNSLs. First, we use different sizes of the same material (e.g. 10.5 nm and 5.6 nm diameter Fe$_3$O$_4$ NPs). Second, we use different materials, such as 14.2 nm Fe$_3$O$_4$ NPs and 6 nm FePt NPs, or 14.2 nm Fe$_3$O$_4$ NPs and 7.1 nm CoPt$_3$ NPs. We observe the formation of large scale BNSLs (up to several µm) due to the high uniformity of these nanoparticles. Using a serial tilting capability of our TEM tomography holder we confirm that the BNSLs are isochemical NaZn$_{13}$ and AlB$_2$ type structures, which are thermodynamically stable due to their high packing density. We further measured the magnetic properties of these BNSLs samples, and single component samples, by SQUID magnetometry. Dipolar and/or exchange coupling between two components is studied.

$^1$Supported by NSF MRSEC DMR-0520020 and ARO/MURI W911NF-08-1-0364.

11:39AM W31.00003 Magnetic domain formation in monolayer nanoparticle films, BRIAN MARANVILLE, KATHRYN KRYCKA, JULIE BORCHERS, National Institute of Standards and Technology, CHARLES HOGG, SARA MAJETICH, Carnegie Mellon University, YUMI IJJIRI, Oberlin College — Self-assembled magnetic nanoparticle films offer promise as data storage media, but an understanding of the interactions is missing. Modified Langmuir-Blodgett methods were used to prepare monolayer films of 7 and 11 nm diameter Fe$_3$O$_4$ nanoparticles with large structural domains. Small-angle neutron scattering (SANS) shows a peak at a wavevector $Q$ corresponding to the particle size and spacing, and scattering at intermediate $Q$ indicating possible long-range correlations. We extend to lower $Q$ with off-specular neutron reflectivity, achieving high intensity by sacrificing resolution along on-plane direction $y$ while retaining high resolution in the other plane direction $x$ and the normal direction $z$. We measure in saturation and zero field to extract magnetic scattering. In high fields, the specular scattering ($Q_y = 0$) is increased, consistent with aligned moments. Preliminary results show weak magnetic scattering for nonzero $Q_z$. Since the maximal $Q_z$ roughly corresponds to the lowest $Q$ in SANS, the combination of these techniques allows us to quantify field-dependent magnetic domain size.
11:51AM W31.00004 Finite size effects and long wavelength magnetic structures in Mn$_3$O$_4$ nanoparticles, R. REGMI, R. TACKETT, G. LAWES, Department of Physics and Astronomy, Wayne State University — Mn$_3$O$_4$ (Hausmannite) having normal spinel structure with Mn$^{2+}$ ion at tetrahedral A site and Mn$^{3+}$ ion at octahedral B site orders ferromagnetically to Yafet-Kittel phase at 42K. The interplay between the different magnetic ions leads to additional magnetic transitions in bulk, including incommensurate and commensurate phases developing at 40K and 34K respectively. We have investigated the magnetic properties of Mn$_3$O$_4$ nanoparticles through both thermodynamic and magnetic studies. Both of these measurements observe only a single magnetic transition at 42K; the transitions at 40K and 34K appear to be completely suppressed. We motivate this suppression by comparing the long wavelength of the magnetic structure in the lower temperature phases with the particle size. These nanoparticles also exhibited superparamagnetic blocking near 40K and frequency dependent magnetic loss at 30K, which we attribute to surface spin effects.

12:03PM W31.00005 Fresnel Lorentz Microscopy Imaging of Domains in Fe3O4 Nanoparticle Arrays, S. A. MAJETICH, E. R. EVARTS, C. HOGG, Physics Department, Carnegie Mellon University, K. YAMAMOTO, T. HIRAYAMA, Japan Fine Ceramics Center — Fresnel Lorentz microscopy was used to study the magnetic domain structures of self-assembled nanoparticle arrays as a function of temperature, from 24 to 605 °C. 11 nm diameter Fe3O4 nanoparticles with an edge-to-edge spacing of 2.5 nm form magnetic domains through magnetostatic interactions alone. At room temperature stripe domains were evident in monolayer arrays. The average domain size in monolayer regions is larger than that in bilayers. Mean field theories predict a reduced stabilization energy for bilayers, relative to that for monolayers. The domain wall positions were fairly stable up to 500 °C, though the contrast in the walls diminished, indicating reduced magnetic order. Above 500 °C there were large temperature-dependent changes. The walls surrounding the smaller domains disappeared at lower temperatures than those of the larger domains. Some magnetic contrast was visible up to 575 °C, close to the Curie temperature of Fe3O4 (585 °C). Transmission electron microscopy after cooling showed that the particle shape and position in the ordered arrays had been preserved during the high temperature imaging experiments.

12:15PM W31.00006 Magnetic imaging of individual nanomagnets, B. KALISKY, J. R. KIRTLLEY, L. QIAN, N. KOSHNIC, Geballe Laboratory for Advanced Materials, Stanford University, M. E. HUBER, Department of Physics, University of Colorado Denver, K. A. MOLER, Geballe Laboratory for Advanced Materials, Stanford University — Characterization of nanomagnets is usually done in ensembles, which is problematic because their magnetic properties are inherently sensitive to small variations in volume, shape and structure. Our aim is to detect and characterize individual nanomagnets using scanning microscopy, which allows gathering statistics about the behavior of many individual particles under the same conditions. Scanning SQUID is a suitable tool for this challenge because it has sensitivity of ~800 spins. We built a scanning microscope for this purpose, which is intended to measure the nanomagnets up to their superparamagnetic state while keeping the SQUID superconducting. We will present on our preliminary efforts to measure FePt particles.

12:27PM W31.00007 FePt nanoparticles as high resolution magnetic force microscope (MFM) probes, LISA QIAN, Stanford University, JAEMIN KIM, Brown University, JOHN KIRTLLEY, BEENA KALISKY, Stanford University, SHOUHENG SUN, Brown University, KATHRYN MOLER, Stanford University — Current MFM probes are often fabricated by sputtering a magnetic thin film across the entirety of an atomic force microscope (AFM) cantilever, limiting their spatial imaging resolution to about 30nm. We report our progress on improving this resolution by using single crystal, high-coercivity ferromagnetic FePt nanoparticles as magnetic sensors for MFM. By attaching nanomagnets 5-10 nm in diameter to the end of a functionalized AFM tip, we have demonstrated that the FePt nanoparticles can be used to achieve atomic resolution in magnetic imaging. The FePt nanoparticles are fabricated by sputtering Fe and Pt onto a Si$_3$N$_4$ cantilever and etching it with a focused ion beam. The FePt nanoparticles are then functionalized with a thin layer of polymer to prevent degradation. The FePt nanoparticles are then attached to the AFM tip using a conductive adhesive.

12:39PM W31.00008 Mechanical Measurement of Magnetization Reversal in a Single Iron Filled Carbon Nanotube, PALASH BANERJEE, M. HERMAN, K.C. FONG, D.V. PELEKHOV, YU. OBUKHOV, P. CHRIS HAMMEL, Dept. of Physics, Ohio State University, 191 W. Woodruff Ave, Columbus OH 43210, F. WOLNY, U. WEISSKER, T. MÜHL, A. LEONHARDT, BERND BÜCHNER, Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstrasse 20, D-01069 Dresden Germany — The hysteresis loop and switching behavior of an individual Fe-filled carbon nanotube (FeCNT) has been measured at low temperatures using cantilever magnetometry. From the magnetometry data, we are able to extract the total moment of the nanotube and the effective anisotropy field arising from the extreme aspect ratio of the nanotube (length ∼ 13 nm, diameter ∼ 25 nm). We have measured the FeCNT’s hysteresis loop and in a single step. These switching fields ($H_s = 2245$ G at 4.2 K) are characterized by a narrow distribution ($\sigma_{sw} \approx 1$ G) and their measured temperature dependence is consistent with a thermally activated process of magnetization reversal. This work was supported by the NSF Materials World Network grant DMR-0807093 and a NSF I2CAM Grant DMR-0645461. P.B. acknowledges support of the ICAM Branches Cost Sharing Fund for a postdoctoral fellowship.

1:03PM W31.00010 Functional nanocomposite polymer films with uniform magnetic nanoparticle dispersions, K. STOJAK, S. PAL, M.J. MINER, H. SRIKANTH, University of South Florida-Physics, S. SKIDMORE, J. WANG, T. WELLER, University of South Florida-Electrical Engineering — Magnetic nanoparticles embedded in polymer matrices are good examples of functional nanostructures with excellent potential in applications such as tunable microwave devices, EMI shielding, and flexible electronics. The challenge comes with evenly dispersing the nanoparticles once they are embedded in the polymer matrix. To avoid clustering of particles in the polymer nanocomposites and achieve excellent dispersion, competition between polymer-polymer and polymer-particle interactions must be balanced. In earlier work, we demonstrated the synthesis of 2 μm thick, spin-coated nanocomposite PMMA films with Fe$_3$O$_4$ (mean size 15nm) nanoparticles embedded that displayed superparamagnetic behavior. In this work we will report on the successful extension of this strategy to 20 μm thick films that are needed for microwave applications. In addition to Fe$_3$O$_4$, we have also functionalized the films with other ferrite nanoparticles. Magnetic characterization and microstructural studies of the polymer nanocomposites will be presented and discussed. Microwave response of these films using a coplanar waveguide fixture will also be reported.
1:15PM W31.00011 Effects of varying surfactant chain lengths on the magnetic, optical and hyperthermia properties of ferrofluids. CORNELIU RABLUI, PREM VAISHNAV, Kettering University, Flint, MI, RAJESH REGMI, CHANDRAN SUDAKAR, CORREY BLACK, GAVIN LAWES, RATNA NAIK, Wayne State University, Detroit, MI, MELISSA LAVOIE, Yale University, New Haven, CT, DAVID KAHN, Oakland University, Auburn Hills, MI — We report studies of the structural, magnetic, magneto-thermal and magneto-optic properties of dextran, oleic acid, lauric acid and myristic acid surfactated Fe$_3$O$_4$ nanoparticles of hydrodynamic sizes ranging from 32 nm to 92 nm. All the samples showed saturation magnetization of ~50 emu/g, significantly smaller than the bulk value for Fe$_3$O$_4$, together with superparamagnetic behavior. The ac magnetization measurements on the dextran coated nanoparticles showed frequency dependent blocking temperature, consistent with superparamagnetic blocking. The ferrofluid heating rates in a 250 Gauss, 100 kHz ac magnetic field varied with the chain lengths of the surfactants, with higher heating rates for longer chains. DC-magnetic-field-induced light scattering patterns produced by two orthogonal He-Ne laser beams passing through the ferrofluid sample revealed different optical signatures for different surfactants.

1:27PM W31.00012 Metallic Iron Nanoparticles for MRI Contrast Enhancement. HAFSA KHURSHID, MICHAEL BONDER, SRINIVASAN BALAKRISHNAN, University of DE, COSTAS HADJIPANAYIS, Emory University School of Medicine, GEORGE HADJIPANAYIS, University of DE — This study is focused on our chemically synthesized iron nanoparticles, coated with carboxyl-methyl terminated polyethylene glycol to make them biocompatible and water dispersible. The particles have an average size of 14 nm and a magnetization of 110 emu/g. TEM studies revealed their core shell structure with iron in the core and iron oxide in the shell. The effects of these nanoparticles on MRI contrast enhancement were studied in vitro using a clinical MRI scanner at a magnetic field of 1.5 T. Both the $r_1$ (1/T$_1$) and $r_2$ (1/T$_2$) were found to be significantly higher than those of iron oxide nanoparticles with a similar size. This behavior is attributed to their stronger magnetic susceptibility, leading to spin dephasing and shortening of T2 effects and thus darkening of the nanoparticles in the MRI contrast. These results suggested that the iron nanoparticles are expected to be more useful for MRI contrast enhancement and other biomedical applications than the currently used iron oxide nanoparticles.

1:39PM W31.00013 RIE-based Pattern Transfer Using Nanoparticle Arrays as Etch Masks. CHIP HOGG, SARA A. MAJETICH, JAMES A. BAIN, Carnegie Mellon University — Nanomasking is used to transfer the pattern of a self-assembled array of nanoparticles into an underlying thin film, for potential use as bit-patterned media. We have used this process to investigate the limits of pattern transfer, as a function of gap size in the pattern. Reactive Ion Etching (RIE) is our chosen process, since the gaseous reaction products and high chemical selectivity are ideal features for etching very small gaps. Interstitial surfactant is removed with an O$_2$ plasma, allowing the etchants to penetrate between the particles. Their pattern is transferred into an intermediate SiO$_2$ mask using a CH$_4$-based RIE. This patterned SiO$_2$ layer is finally used as a mask for the MeOH-based RIE which patterns the magnetic film. We present cross-sectional TEM characterization of the etch profiles, as well as magnetic characterization of the film before and after patterning.

1:51PM W31.00014 Magneto-Transport in quantum dot films. ALEXANDRE POURRET, PHILIPPE GUYOT-SIONNET, James Franck Institute, The University of Chicago — Colloidal semiconductor quantum dots are being studied intensely because of their tunable optical properties. Quantum dot solids (e.g. films) present further interesting possibilities for designing novel materials with control of the electronic properties at the nanometer scale. While neutral CdSe or CdSe/CdS nanocrystal films are quite insulating, photo excitation or doping the film electrochemically leads to higher conductivity. In this talk I will present photocconductivity and conductivity measurements of charged CdSe and CdSe/CdS nanocrystal films at low temperature under a magnetic field. The combination of electrochemistry and spectroscopy enables the precise control and detection of electrons injected into the quantum dot films. The temperature and electric field dependent conductivity is analyzed with the variable range hopping model of Efros and Shklovskii and the magneto-conductivity is discussed in terms of a spin-blockade.

2:03PM W31.00015 Surface and Size Manipulation of the Magnetic Properties of CdSe Quantum Dots. ROBERT MEULENBERG, Laboratory for Surface Science and Technology and Department of Physics and Astronomy, University of Maine, JONATHAN LEE, SCOTT MCCALL, LOUIS TERMINELLO, TONY VAN BUUREN, Lawrence Livermore National Laboratory — The appearance of magnetism in otherwise non-magnetic materials has recently been reported for a number of nanoscale materials. Coupled with the size-dependent optical and electronic properties of the nanocrystalline materials, this magnetic behavior opens the possibility for an extended range of technological applications. As such, identifying the origin of the magnetism is an extremely important goal, yet this remains the subject of some controversy in the literature. We report evidence that paramagnetism in CdSe QDs can be induced via manipulation of the particle size and surface ligands. Using SQUID magnetometry and x-ray absorption spectroscopy, we demonstrate that the paramagnetic behavior of the CdSe QDs can be varied by changing the ligand endgroup functionality of the passivating layer. Contrary to previous reports, no evidence for ferromagnetism was observed.

3This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.


11:15AM W32.00001 The Ising model for the bcc, fcc and diamond lattices; a comparison. PER HÅKAN LUNDOW, KTH, KLAS MARKSTRÖM, Umeå University, ANDERS ROSENGREN, KTH — A large scale Monte Carlo simulation study of the Ising model for the simple cubic lattice was recently performed (Adv. Phys. 56, 653–755 (2007)). We have complemented that with a study of the bcc, fcc and diamond lattices. Both the canonical and microcanonical ensembles were employed. We present estimates of the critical temperature and other quantities in the critical region. An analysis of the critical behaviour suggests distinct high- and low-temperature exponents, especially for the specific heat, as was obtained also for the simple cubic lattice. This discrepancy is briefly discussed.

3Supported in part by the Swedish Research Council
11:27AM W32.00002 Thermodynamicsof magnetic systems from first principles: gWL-LSMS 1, MARKUS EISENBACK, G. MALCOLM STOCKS, DON M. NICHOLSON, THOMAS SCHULTHES, Oak Ridge National Laboratory — Density Functional Calculations have proven to be a useful tool to study the ground state of many materials. For finite temperatures the situation is less ideal an one is often forced to rely on models with parameters either fitted to first principles or experimental results. This approach is especially unsatisfactory in inhomogeneous systems, nano particles or other systems where the model parameters should vary significantly from one site to another. Here we describe a possible solution to this problem by combining classical thermodynamic Monte Carlo calculations - The Wang-Landau method in this case [F Wang and DP Landau, PRL 86, 2050 (2001)] - with a first principles electronic structure calculation, specifically our locally selfconsistent multiple scattering code. The combined code shows superb scaling behavior on massively parallel computers and first tests on Fe systems provide a proof of principle.

1Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

11:39AM W32.00003 Quantum Monte Carlo calculates bulk properties and magnetic ordering in iron 1, WILLIAM D. PARKER, JOHN W. WILKINS, Ohio State University — Quantum Monte Carlo (QMC) models electronic systems with high accuracy but its computational demands limit wider use. Few QMC calculations exist for solid-state systems and none comparing the energetic ordering of different spin configurations (magnetic states). Density-functional calculations with generalized-gradient-approximation exchange-correlation give correct magnetic ordering and accurate lattice constants and bulk moduli for bcc iron. However, the predicted cohesive energy differs from experiment by 0.5-1.0 eV. QMC-calculated bulk elastic properties for pure iron in the bcc, hcp and fcc phases compare with properties in the ferromagnetic, antiferromagnetic and nonmagnetic spin configurations.

1The Ohio Supercomputing Center, NERSC and CCNI gave computational support. The DOE provided financial support(DE-FG02-99ER45795).

11:51AM W32.00004 Current-driven vortex oscillations in metallic nanocontacts, GINO HRKAC, University of Sheffield — In this paper, we performed full micromagnetism simulations of metallic nano-contacts from the TUNAMOS consortium, by solving the Landau Lifshitz Gilbert Slonctewski equation simultaneously with quasi-static Maxwell equations. We take into account the spatially inhomogeneous current distribution flowing through the magnetic free layer and consequently use the Oersted field generated by this current for the magnetization dynamics. The system we simulated was a 40nm-CoFe 2.5nm/Cu 3nm/NiFe 4nm stack. The saturation magnetization of the free layer is taken to be the same as the experimental value Ms = 1.1 T, and a GMR ratio of 1% is used. We account for the inhomogeneous current distribution flowing through the free layer by computing the local current density from the local angle between the free and fixed layer magnetizations. The Oersted field is computed with the Biot-Savart law from this current distribution [2], and an asymmetric Sloncetzewski term for the spin transfer is used [3]. We observe that the additional spin torque drives the vortex out of the contact area and towards a stable orbit around the contact. These simulations reveal that the oscillations observed are related to the large-amplitude translational motion of a magnetic vortex. In contrast to the nanopellar geometry in which the vortex core precesses within the confining part of the Oersted field [1], the dynamics here correspond to an orbital motion outside the contact region. This behavior can be likened to planetary orbital motion under the influence of a gravitational field; the spin-transfer torque leads to a centripetal motion of the vortex core, which is counterbalanced by the attractive potential provided by the Oersted field. Good quantitative agreement between the simulation and experimental frequencies is achieved [4].


12:27PM W32.00005 Monte Carlo simulation of incommensurate helical ordering in a frustrated FCC lattice of Heisenberg spins, SEONGWEON PARK, CH. M. SULLIVAN, G. SCHNEIDER, T.M. GIEBULTOWICZ, Oregon State University — The zinblende structure of MnSe can be stabilized in thin films and is expected to exhibit Type III FCC antiferromagnetic ordering. The expected magnetic order is indeed observed in MnSe/ZnSe superlattices where the MnSe layers experience compressive strain. However, in the MnSe/ZnTe system, in which MnSe layers experience tensile strain, the Mn spins form incommensurate helical structures [1]. Mean field theory can explain the basic mechanism leading to helical ordering but cannot explain details such as the temperature dependence of the pitch of the helical ordering. We report results of Monte Carlo simulations using classical 3D Heisenberg spins and “free” boundary conditions. The simulations were performed for a range of systems with different sizes (including “bulk” thickness) and exchange constants. The change of helical pitch with temperature is correctly reproduced in our results and our data indicate that it is at least partially a finite-thickness effect. We compare our results with earlier simulations using XY spins and “self-determined” boundary conditions [2].


12:39PM W32.00006 Dynamical magnetizations of nanomagnets with strong magnetic anisotropy, BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We developed a non-equilibrium Monte Carlo method to investigate dynamical spins and magnetizations of nanomagnets with strong magnetic anisotropy and applied it to Co spin chains on Pt surface and a composite spin system (Phys. Rev. B 73, 174418; Phys. Rev. Lett. 96, 217201; Front. Phys. China 2, 424). Here we report on our exploration for universal dynamical magnetic properties of spin chains and single-layered nanomagnets with strong magnetic anisotropy. Furthermore, we investigate representative systems composed of sub-10nm nanomagnets with large uniaxial anisotropy for magnetic data storage, finding various magnetization memory effects and aging effects in such single systems of the interacting nanomagnets with the same easy axis, and study the exchange bias and training effect observed in composite films and heterostructures. This method is proved to be effective and reliable in simulating dynamical magnetism in nanomagnets with strong magnetic anisotropy.

13:51PM W32.00007 Tailoring Effective Exchange Interactions via Domain Walls in Coupled Heisenberg Rings, VANITA SRINIVASA, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260 — The nature of the exchange coupling variation in an antiferromagnetic spin-1/2 system can be used to tailor its ground-state properties. In particular, dimersed Heisenberg rings containing domain walls have localized states which can serve as “flying spin qubits” when the domain walls are moved (PRB 76, 094411 (2007)). We show theoretically that, when two of these rings are coupled, the movement of the domain walls leads to modulation of the effective exchange interaction between the qubits. Appropriately chosen configurations of domain walls can give rise to ferromagnetic effective exchange. We describe how these spin rings may be used as basic building blocks to construct quantum spin systems whose properties are tunable by virtue of the exchange variation within the rings.

1This work was supported by a NDSEG fellowship (VS) and the Department of Energy, Basic Energy Sciences (DE-FG02-07ER44621).
1:03PM W32.00008 Electron magnetism of antiferromagnetic conductors,1, REVAZ RAMAZASHVILI, LPTMS, Orsay — Essential momentum dependence of the electron g-tensor in an antiferromagnet turns the common Zeeman term into a spin-orbit coupling. I will discuss some of the remarkable experimental consequences of this phenomenon. The predictions may be relevant to antiferromagnetic conductors from chromium to electron- and hole-doped cuprates, borocarbides, pnictides, organic and heavy fermion materials.

1I thank LPTMS for the kind hospitality, and IFRAF for generous support.

1:15PM W32.00009 On the Electric-Field-Controlled Surface Ferromagnetic Transition in Metals1, IGOR V. OVCHINNIKOV, KANG L. WANG, UCLA, E&E DEPT., DRL TEAM — It is widely believed that in metals, unlike in the dilute magnetic semiconductors, the control of the ferromagnetic ordering by an external voltage is hardly achievable. We compare the two materials and show that there is no obvious reason why metals are less preferable for this phenomenon. Similar effect in metals, however, has a different physical picture and should be identified as a voltage-induced surface ferromagnetic transition. We study its properties within the theory of the surface critical phenomena and discuss possible difficulties on the way to its experimental realization.

1The work was supported in part by Western Institute of Nanoelectronics at UCLA.

1:27PM W32.00010 Effect of fluctuations on effective Hamiltonians of anisotropic frustrated pyrochlore antiferromagnets,2, PAUL MCCLARTY, MICHEL GINGRAS, University of Waterloo — The rare earth pyrochlore magnets $\text{R}_2\text{Ti}_2\text{O}_7$ exhibit a wide range of puzzling features. $\text{R}_2\text{Ti}_2\text{O}_7$, a weakly Ising-like antiferromagnet, is a cooperative paramagnet down to, at least, 50 mK despite having a ~20 K Curie-Weiss temperature. $\text{Er}_2\text{Ti}_2\text{O}_7$, which has magnetic ions with a strong easy plane anisotropy, has a transition to an ordered phase but the origin of a long-range ordered state with discrete broken symmetry is not understood. Recent experimental work has also uncovered interesting field-induced phases in both of these materials. We construct effective Hamiltonians, derived from microscopic models, for these two frustrated antiferromagnets by considering the effects of quantum fluctuations out of the classical ground states of these models to assess the stability of these states, the nature of the excitations and possible mechanisms of degeneracy breaking.

1:39PM W32.00011 Ferromagnetic spin coupling as the origin of 0.7 anomaly in quantum point contacts1, KARAN ARYANPOUR, JONG E. HAN, Department of Physics, SUNY at Buffalo — We study one-dimensional itinerant electron models with ferromagnetic coupling to investigate the origin of 0.7 anomaly in quantum point contacts (QPC). Linear conductance calculations using the Kubo formula from the quantum Monte Carlo (QMC) technique for spin interactions of different spatial range suggest that 0.7 x $(2e^2/h)$ anomaly results from a strong interaction of low-density conduction electrons to ferromagnetic fluctuations formed across the potential barrier. The conductance plateau results due to the strong incoherent scattering at high enough temperatures when the electron traversal time through the gate voltage barrier matches the time-scale of dynamic ferromagnetic excitations (magnons). In addition, our model also captures the correct evolution of the anomalous plateau as a function of temperature and Zeeman magnetic field.

2This project was supported by NSF DMR-0426826 and we acknowledge the CCR at the SUNY Buffalo for computational resources.

1:51PM W32.00012 Intrinsic Perturbation of the Landau Levels in Metals and Semiconductors at Low Temperatures, AYODEJI AWOBODE, University of Illinois at Urbana Champaign — The de Haas–van Alphen effect in non-superconducting metals and semiconductors at very low temperatures is proposed as a test of an intrinsic perturbative term which appears in the Landau equation sequel to the modification of the Pauli equation. Corrections to the frequency (or period) of the de Haas–van Alphen oscillation in metals is calculated and shown to depend on the Fermi energy and the measured anomalous part of the electron magnetic moment. Precision measurement of the magneto-optical properties which arise from the motion of electrons in binary semiconductors placed in a weak magnetic field is also proposed as a means of observing very small changes in the relationship between current I and magnetic field H derived from Ampere’s Law is $H = \frac{N I}{L}$, where $N I$ is magnetomotive force and $L$ is the length of the magnetic path. However, this formula fails to describe the variation in magnetic field with position. In fact H is usually inhomogeneous around a closed path unless special precautions have been taken to ensure uniformity. In order to describe the magnetic field around a closed circuit we have introduced extensions to the standard formula for a finite coil in a closed circuit. This includes parameters for location and shape of core to enhance the accuracy. This analytic model produces fast and accurate predictions for the variation of H with position. Results are comparable with FEM calculations that take much longer to generate.

2:03PM W32.00013 Variation of magnetic H field in closed loop magnetic circuits: problems with the standard equation, ESAINDANG UMENEI, EUGENE MELIKHOV, DAVID JILES, Wolfson Centre for Magnetics, Cardiff University, WOLFSOON CENTRE FOR MAGNETICS TEAM — We have developed a reliable method for calculating the variation of magnetic field H in closed circuits. This offers advantages over standard numerical Finite Element Modeling which requires meshing of the spatial domain. Such calculations can consume enormous computational resources and time. Analytical models work much faster but are only applicable in restricted cases. The well known “standard model” for the relationship between current I and magnetic field H derived from Ampere’s Law is $H = \frac{N I}{L}$, where $N I$ is magnetomotive force and $L$ is the length of the magnetic path. However, this formula fails to describe the variation in magnetic field with position. In fact H is usually inhomogeneous around a closed path unless special precautions have been taken to ensure uniformity. In order to describe the magnetic field around a closed circuit we have introduced extensions to the standard formula for a finite coil in a closed circuit. This includes parameters for location and shape of core to enhance the accuracy. This analytic model produces fast and accurate predictions for the variation of H with position. Results are comparable with FEM calculations that take much longer to generate.

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11:15AM W33.00001 Mott transition, magnetism and d-wave superconductivity on lattices with frustration1, A.M.-S. TREMBLAY, BUMSOO KYUNG, Universite de Sherbrooke — By tuning band parameters and choosing appropriate lattices, it is possible to frustrate antiferromagnetism to reveal the competing d-wave superconducting (d-SC) phase, the normal phase and the Mott insulating phase. We study the nature of the competition between these phases by using Cellular Dynamical Mean-Field Theory for the Hubbard model on the anisotropic triangular lattice and on the square lattice with second-neighbor hopping. The phase diagram in the $T = 0$ plane is drawn as a function of interaction strength $U/t$ and frustration $t'/t$. The critical interaction strength for the Mott transition is found as a function of frustration. At half-filling and for intermediate coupling we find that outside the Mott insulating phases, d-SC appears at an optimal level of frustration. We also identify spin fluctuations as the source of pair formation. We find that components of the spin susceptibility involved in binding are mostly centered in the quarter of the Brillouin zone closest to $(\pi, \pi)$. We conclude that retarded short-range spin fluctuations are crucial for d-SC even in the presence of frustration and that there are optimal values of frustration that favor d-SC.

1NSERC, CRC, CFI, CIFAR.
11:27AM W33.00002 Superconductor-Metal-Insulator Phase Transition in Ta Films. YIZE LI, JONGSOO YOON. University of Virginia — We have reported the magnetically induced metallic phase in superconducting Ta films which intervenes the superconducting and insulating phases [1]. Recently, we studied the electronic transport properties of Ta film with various degrees of disorders which were controlled by film thickness. We found that as sample thickness decreases, the films undergo a superconductor-metal-insulator phase transition. Each phase exhibits distinct nonlinear current-voltage (I-V) characteristics, similar to those of magnetically induced superconductor-metal-insulator transition. We have measured the evolution of nonlinear I-V with changing magnetic field (B) and temperature (T), for representative samples with different degrees of disorders, which leads to the phase diagram in B-T-Disorder space. [2] Y.Qin et al., Phys. Rev. B 73, 100505(R) (2006).

11:39AM W33.00003 Dissipation-driven quantum phase transition in superconductor-graphene systems1 . ROMAN LUTCHYN, VICTOR GALITSKI, University of Maryland. GIL REFAEL, California Institute of Technology, SANKAR DAS SARMA, University of Maryland — We show that a system of Josephson junctions coupled via low-resistance tunneling contacts to graphene substrate(s) may effectively operate as a current switching device. The effect is based on the dissipation-driven superconductor-to-insulator quantum phase transition, which happens due to the interplay of the Josephson effect and Coulomb blockade. Coupling to a graphene substrate with gapless excitations further enhances charge fluctuations favoring superconductivity. The effect is shown to scale exponentially with the Fermi energy in graphene, which can be controlled by the gate voltage. We develop a theory, which quantitatively describes the quantum phase transition in a two-dimensional Josephson junction array, but it is expected to provide a reliable qualitative description for one-dimensional systems as well. We argue that the local effect of dissipation-induced enhancement of superconductivity is very robust and a similar sharp crossover should be present in finite Josephson junction chains.

1This work is supported by JQI and US-ONR

11:51AM W33.00004 Superfluid response of a gated LaAlO3 / SrTiO3 heterostructure. SHASHANK MISRA, LUKAS URBAN, STEFAN THIEL, CHRISTOPH RICHTER, GERMAN HAMMERL, JOCHEN MANNHART, Universität Augsburg, ALI YAZDANI, Princeton University — Disordered two-dimensional superconductors undergo a quantum phase transition into an insulating phase, with an unusual intervening metallic phase, upon the introduction of sufficiently large amounts of disorder or the application of a sufficiently strong magnetic field. The LaAlO3 / SrTiO3 heterostructure, because it can be gated, provides a new opportunity: to see how two-dimensional superconductivity is destroyed continuously as a function of carrier concentration. We build on the electrical transport measurements in other works, which demonstrated the existence of a superconductor-insulator transition upon decreasing the carrier concentration, by using a two coil mutual inductance technique to measure the complex ac conductivity. We will track the superfluid density, which can be derived from the complex conductivity, throughout parts of the carrier concentration-temperature-magnetic field phase diagram, and make comparisons with data from the field-tuned superconductor-insulator transitions in MoGe and InOx. This work is supported by the DOE and the DFG via SFB484.

12:03PM W33.00005 Giant enhancement of superconductivity in ultrathin α-Pb films by a parallel magnetic field: effect of magnetic impurity. ASHWANI KUMAR, H. JEFFREY GARDNER, LIQUI YU, PENG XIONG, Department of Physics and MARTECH, Florida State University — An ultrathin superconductor containing paramagnetic impurities is predicted1,2 to exhibit enhancement of superconductivity (TC and IC) when subject to a parallel magnetic field. We have recently observed a pronounced enhancement of superconductivity in ultrathin homogeneous amorphous Pb films without any (intentionally added) magnetic impurities in the presence of a parallel magnetic field; the TC enhancement is as large as 13% and persists in field as high as 8 T. Our experiments are carried out in a modified dilution refrigerator capable of situ film growth, sample rotation, and incremental deposition of magnetic (Cr) impurities, which allows for a systematic, unambiguous elucidation of the effect of paramagnetic impurities on the field-enhancement of superconductivity. With increasing Cr density on a Pb film, the magnitude of the TC enhancement is progressively suppressed, contrary to the theoretical predictions. 1 Khartonov et al., JETP Lett. 82, 473 (2005). 2 Wei et al., Europhys. Lett. 75, 943 (2006).

12:15PM W33.00006 A direct transition between a Neel ordered Mott insulator and a dx2−y2 superconductor on the square lattice. YING RAN, ASHVIN VISHWANATH, DUNG-HAI LEE, UC Berkeley — In this paper we study a bandwidth-controlled direct, continuous, phase transition from a Mott insulator, with easy plane Neel order, to a fully gapped dx2−y2 superconductor with a doubled unit cell on the square lattice, a transition that is forbidden according to the Landau paradigm. This transition is made possible because the vortices of the antiferromagnet are charged and the vortices of the superconductor carry spins. These nontrivial vortex quantum numbers arise because the ordered phases are intimately related to a topological band insulator. We describe the lattice model as well as the effective field theory.

12:27PM W33.00007 Superconductor to Quantum Metal Transitions in Ultra Thin Films1 . YEN-HSIANG LIN, ALLEN M. GOLDMAN, University of Minnesota — Homogeneous films of amorphous bismuth have been continuously tuned from the superconducting state by increasing a perpendicular magnetic field. Electrical transport and Hall measurements show that the non-superconducting states of the films are quantum-corrected metals. In the vicinity of transition field, the resistance can be fit by an Arrhenius type of conduction at high temperatures but this form fails at lower temperatures where the resistance is a non-monotonic function of temperature. This suggests that a two-phase regime develops near criticality. Theories suggest that this is in the form of superconducting puddles embedded in a normal matrix1,2. 1B. Spivak, P. Oreo, and S. A. Kivelson, Phys. Rev. B 77, 214523 (2008) 2Y. Dubi, Y. Meir, and Y. Avishai, Nature 449, 876-880 (2007)

1This work is supported in part by the National Science Foundation under grant NSF/DMR-0455121.

12:39PM W33.00008 The superconductor-insulator transition: is there a new insulating state? MAOZ OVADIA, BENJAMIN SACEPE, DAN SHAHAR, Weizmann Institute, Israel — We present nonlinear conductivity measurements on the insulating side of the superconductor-insulator transition in amorphous indium oxide. The results agree with previous data1,2, and show conductance jumps at well-defined voltage bias thresholds. The current in the sample changes by as much as a factor of 105 at the threshold, from our noise floor of 3×10−14A to over 10−8A. The jumps disappear above a magnetic-field- dependent temperature TC, which is 0.11K or lower. The threshold voltage changes from 20μV to over 0.2V (4 orders of magnitude) by application of a magnetic field. We ask whether a true zero conductance state exists in our samples. DC measurements reveal pseudo-exponential I-V characteristics, which can be extrapolated to find the high Ohmic resistance of these samples at low temperatures. The extrapolated R(T) curves typically show a sub-activated trend at low T. Our results suggest that our samples have zero conductance only at the absolute zero of temperature.

(1) Sambandamurthy et al. PRL 92, 107005
(2) Baturina et al. Nature Letters 452, p613
12:51PM W33.00009 Metal-insulator transition and superconductivity in the Mott insulator GaTa\textsubscript{2}Se\textsubscript{8} : towards a tuning of the Mott transition by electric pulses, E. JANOD, C. VALIU, IMN, V. DUBOST, INSP, B. CORRAZE, IMN, T. CREN, INSP, P. MOREAU, IMN, F. DÉBONTRIDDER, INSP, D. BRATHWAITE, CEA Grenoble, D. RODITCHDEV, INSP, L. CARIO, IMN, TEAM, INSP TEAM, CEA GRENoble TEAM — We have recently discovered the existence of a non-volatile electric-pulse-induced resistive switching (EPI-RS) in the spinel Mott insulator GaTa\textsubscript{2}Se\textsubscript{8} [1]. The origin of this effect is different from other EPI-RS mechanisms identified to date [2]. A granular superconducting state below $T_C = 5$ K, ascertainment by critical current and critical field data obtained on single crystals, appears in the EPI "metallic" state. This transition is reminiscent of the bulk superconductivity at 5-8 K obtained under pressure [3]. Interestingly, STM experiments have revealed a puzzling electromechanical coupling between the tip voltage and the GaTa\textsubscript{2}Se\textsubscript{8} sample surface. All these results may therefore indicate that, beside electronic doping and pressure, electric pulses, through an electrostrictive effect, could be a relevant parameter to tune the Mott metal-insulator transition. [1] C. Vajú et al., Adv. Mater. 20, 2760 (2008) [2] R. Waser, M. Aono, Nature Mat. 6, 833 (2007) [3] M.M. Abd-Elmeguid et al., PRL 93, 126403 (2004)

1:03PM W33.00010 Enhanced Suppression of Superconductivity in Amorphous Films with Nanoscale Patterning, VADIM OGANESYAN, CUNY Staten Island, SHIVAJI SONDHI, Princeton University — We discuss the superconductor to normal phase transition in an array of small Josephson junctions driven by an applied current. The approach is a generalization of one previously used to treat the metastable superconducting state in an array of small Josephson junctions driven by an applied current. The approach is a generalization of one previously used to treat such an array at zero applied current. The array Hamiltonian is treated variationally using the Gibbs-Bogoliubov inequality, using a set of harmonic "phase phonons" as the variational state. We find that, for a given $J/U$, where $J$ and $U$ are the Josephson and charging energies, a superconducting (S) to insulating (I) transition occurs as a function of applied current, or by varying the direction of the applied current at fixed magnitude. The critical values of $J/U$ are calculated for a square, triangular, and simple cubic lattices of Josephson junctions as a function of bias current. The resulting critical $J/U$ is found to be non-monotonic with the film thickness. We have observed a pronounced enhancement of superconductivity in ultrathin 3-Pb films in the presence of a parallel magnetic field. We have measured the transition temperature of the superconducting critical temperature, $T_c(d_{xy})$, in amorphous Bi/Sb films patterned with a regular array of holes as well as nanoscale thickness variations. We find that the mean field $T_c$ is suppressed relative to simultaneously produced unstructured films of the same thickness. Surprisingly, however, the functional form for $T_c(d_{xy})$ remains unaffected. The role of the thickness variations in suppressing $T_c$ is compared to the role of the holes, through parameterization of the surface, as measured through AFM/SEM and a proximity effect calculation. These results suggest that these two nanoscale modifications suppress $T_c$ about equally and are consistent with $T_c$ being determined on a microscopic length scale.

1This work supported by the NSF through DMR-0203608 and No. DMR-0605797, by the AFRL, and by the ONR.

1:15PM W33.00011 Giant enhancement of superconductivity in ultrathin a-Pb films by a parallel magnetic field: effect of film thickness, H. J. GARDNER, L. YU, A. KUMAR, P. XIONG, Florida State University — We have measured the thickness dependence of the superconducting critical temperature, $T_c(d_{xy})$, in amorphous Bi/Sb films patterned with a regular array of holes as well as nanoscale thickness variations. We find that the mean field $T_c$ is suppressed relative to simultaneously produced unstructured films of the same thickness. Surprisingly, however, the functional form for $T_c(d_{xy})$ remains unaffected. The role of the thickness variations in suppressing $T_c$ is compared to the role of the holes, through parameterization of the surface, as measured through AFM/SEM and a proximity effect calculation. These results suggest that these two nanoscale modifications suppress $T_c$ about equally and are consistent with $T_c$ being determined on a microscopic length scale.

1:27PM W33.00012 Superconductor-insulator transitions in films patterned with a disordered nanohoneycomb hole array, H. Q. NGUYEN, S. M. HOLLEN, M. D. STEWART, JR., AIJUN YIN, J. M. SHAINLIN, J. M. XU, J. M. VALLES, JR., Brown University — On both sides of the Superconductor-Insulator Transition (SIT), ultrathin Bi films patterned with an ordered array of holes exhibit magnetoresistance (MR) oscillations with a period set by the superconducting flux quantum[1]. This observation implies that the insulating phase consists of localized Cooper pairs. To probe further this localized Cooper pair phase we have investigated samples patterned with disordered hole arrays. We have found that disorder reduces the number of MR oscillations and weakens the magnetic field tuned SIT. We will present these results and discuss their implications for the Cooper pair insulating phase.


1This work was supported by the NSF through No. DMR-0203608 and No. DMR-0605797, by the AFRL, and by the ONR.

1:39PM W33.00013 High field magnetoresistance peak near the superconductor-insulator transition in amorphous Bi films patterned with a nanohoneycomb array of holes, S. M. HOLLEN, H. Q. NGUYEN, M. D. STEWART, JR., J. M. SHAINLINE, AIJUN YIN, J. M. XU, J. M. VALLES, JR., Brown University — The spectacular magnetoresistance (MR) peak that appears on the insulating side of the Superconductor-Insulator Transition (SIT) in In Oxide films [1] has received much attention. It has been taken as a sign that Cooper pairs persist into their insulating phase. We have observed a similar MR peak in ultrathin amorphous Bi films patterned with a disordered nanohoneycomb array of holes. This peak increases in magnitude with decreasing thickness and moves to lower field with decreasing temperature. Most importantly, it coexists with MR oscillations at lower fields that reveal the presence of Cooper pairs [2]. We will present our latest investigations of this peak and contrast our results with the behavior of unpatterned amorphous film systems.


This work was supported by the NSF through No. DMR-0203608 and No. DMR-0605797, by the AFRL, and by the ONR.

1:51PM W33.00014 Superconductor-Insulator Phase Transitions in Current-Biased Arrays of Small Josephson Junctions, CHRISTOPHER PORTER, DAVID STROUD, The Ohio State University — We present a variational approach to treat the metastable superconducting state in an array of small Josephson junctions driven by an applied current. The approach is a generalization of one previously used to treat such an array at zero applied current. The array Hamiltonian is treated variationally using the Gibb's-Bogoliubov inequality, using a set of harmonic "phase phonons" as the variational state. We find that, for a given $J/U$, where $J$ and $U$ are the Josephson and charging energies, a superconducting (S) to insulating (I) transition occurs as a function of applied current, or by varying the direction of the applied current at fixed magnitude. The critical values of $J/U$ are calculated for a square, triangular, and simple cubic lattices of Josephson junctions as a function of bias current. The resulting critical $J/U$ is found to be highly sensitive to changes in bias current magnitude, and somewhat less sensitive to current direction, for all geometries studied.

[1] Work supported in part by NSF DMR04-13395

2:03PM W33.00015 Biot-Savart correlations in layered superconductors, KUMAR RAMAN, UC Riverside, VADIM OGANESEYAN, CUNY Staten Island, SHIVAJI SONDHI, Princeton University — We discuss the superconductor to normal phase transition in an infinite layered type-II superconductor in the limit where Josephson coupling between layers is negligible. We model each plane as a neutral gas of thermally excited pancake vortices and assume the Biot-Savart interaction between vortices is the dominant mechanism for coupling the layers. Using the real-space renormalization group, we demonstrate that the transition in this model is a Kosterlitz-Thouless transition driven by the unbinding of pancake vortices. We study the high temperature phase using a Debye-Huckel type mean field theory. We find that while the long range interaction leads to correlations between the planes, the screening within the individual layers is not significantly different from an isolated two-dimensional system. This overall picture places some claims expressed in the literature on a more secure analytical footing and also resolves some conflicting views. Experimental implications will be discussed.
temperatures, which depended upon the applied current. At this writing, the origin of the effect is unclear. This negative magnetoresistance can be as large as 50 percent even with applied field as low as few Oersted. This effect was found over a narrow range of temperatures, which depended upon the applied current. At this writing, the origin of the effect is unclear.

11:27AM W34.00002 ABSTRACT WITHDRAWN

11:39AM W34.00003 Electronic structure of quasi-one-dimensional edge-sharing cuprate LiCu$_2$O$_2$ single crystals measured by angle-resolved photoemission spectroscopy, K.-D. TSUEI, C.-M. CHENG, J.-Y. YUH, National Synchrotron Radiation Research Center, Hsinchu, Taiwan R.O.C., K.W. YEH, M.K. WU, Insitute of Physics, Academia Sinica, Taipei, Taiwan, R.O.C. — We have carried out a high resolution angle-resolved photoemission study on edge-sharing quasi-one-dimensional (1D) chain cuprate LiCu$_2$O$_2$ single crystals at room temperature. The low energy electron diffraction of cleaved (001) surfaces show a well ordered (2x1) pattern with single domain. Absence of photon energy dependence of high lying peaks just below the Fermi energy in the normal emission spectra suggests localization within the ab-pannar layers. One can identify three dispersive bands between 0.5 eV and 2 eV binding energies along the high symmetry directions along with the off-normal spectra. The highest energy peak is observed at the Y-point with a binding energy 0.55 eV bearing a d$_{xy}$ symmetry based on a polarization dependent selection rule, and can be associated with a hybridized state of primarily Cu 3d$_{xy}$ and O 2p orbitals, in agreement with a LDA band calculation. We observed no indication of a band maximum at half integral position along GY, predicted by a 1D $t-J$ model. Another peak at 1.3 eV shows a strong dispersion along GY, normal to the chain direction. Its identity will also be discussed.

11:51AM W34.00004 Synthesis and characterization of superconducting, single-crystal Al nanowires using template based electrodeposition. MEENAKSHI SINGH, JIAN WANG, MINGLIANG TIAN, Penn State University, ALEXIS PEREIRA, University of Puerto Rico Cayey, NITESH KUMAR, THOMAS MALLOUK, MOSES CHAN, Penn State University — Al nanowires (ANW) have been fabricated using template based electrodeposition at room temperature for the first time. An anhydrous electrolyte comprised of AlCl$_3$ and LiAlH$_4$ in tetrahydrofuran with a Pt anode and Ag cathode was used to electrodeposit Al in an anodic aluminum oxide template. X-ray diffraction and electron diffraction show that the ANW are single crystal with (110) as the growth direction. Transmission electron microscopy shows that the wires have uniform diameters with an oxidation layer a few nanometers thick around them. Four electrode transport measurements on a single 70 nm thick ANW have shown significant enhancement in the critical temperature and the critical field and decrease in the critical current density from the bulk value.

11:03PM W34.00005 Resistance in Superconducting Epitaxial Niobium Nanowires and Films, TIMOTHY MCARDLE, ALLISON DOVE, KEVIN INDERHEES, MITRABHANU SAHU, ALEXEY BEZRYADIN, PAUL GOLDBART, JAMES ECKSTEIN, Univ of Illinois, Urbana-Champaign — The thermally activated phase slip (TAPS) description of resistance in one-dimensional superconducting wires is unable to explain additional resistance observed in extremely narrow nanowires well below the critical temperature. We fabricate nanowires using electron beam lithography from single-crystal niobium films grown by ultra-high vacuum molecular beam epitaxy. Since the resulting wires are single crystal and homogenous, the role of disorder is reduced and neither weak links nor grains are present. The epitaxial films are 10 to 30 nm thick, while the finished wires range in length from 1 to 10 µm, and in width from 35 to 200 nm. Transport measurements on the nanowires of varying widths show a range of distinct temperature dependencies below the critical temperature that cannot be accounted for by the single exponential form of the TAPS model.

12:15PM W34.00006 Two superconducting transitions and periodic magnetoresistance oscillations in the crystalline Au nanowire with superconducting electrodes, JIAN WANG, CHUNTAI SHI, MINGLIANG TIAN, JAINENDRA JAIN, QI ZHANG, NITESH KUMAR, MEENAKSHI SINGH, THOMAS MALLOUK, MOSES CHAN, Penn State University — Transport measurements were made on individual crystalline Au nanowire with four focused ion beam (FIB) deposited tungsten (W) electrodes, which are superconducting below 5 K. It was found that the 1.2 microns long (between the inner edges of the two voltage electrodes) Au nanowire is superconducting. Instead of a single sharp drop to zero resistance as seen in usual superconductors, here the resistance drops in two steps. Below TC, with a magnetic field applied perpendicular to the axis of the nanowire, we found “magnetoresistance mini-gaps” in low field regime. In addition, clear periodic magnetoresistance oscillations in the superconducting to normal transition region were observed. All the 1 micron and 1.9 microns Au nanowires were also investigated to further reveal the anomalous superconductivity we found.

Work supported by NSF MRSEC program under grant DMR-0820404.

12:27PM W34.00007 Vortext blockade and conductance fluctuations of superconducting strips in magnetic fields, PAUL GOLDBART, University of Illinois at Urbana Champaign, GIL REFAEL, California Institute of Technology, DAVID PEEKER, Harvard University — Recent experiments on the conductance of a thin, narrow superconducting strip found periodic fluctuations as a function of the perpendicular magnetic field, with the period corresponding to approximately two flux quanta per strip area [1]. Using vortex-charge duality, we explore the possibility that the superconducting strip is the dual of a quantum dot, with vortices playing the role of the electrons, the magnetic field appearing as the gate voltage, and the applied current replacing the source-drain voltage. As with a quantum dot, extrema of the conductance are obtained when configurations with $n$ and $n+1$ vortices have equal energy; in the bias-current versus magnetic-field plane, the conductance displays blockade diamonds. Furthermore, we find that there is a simple relation between the linear-response conductance and the critical current, as they are both set by the barrier to vortex tunneling on to and off of the strip. [1] A. Johansson et al. Phys. Rev. Lett. 95, 116805 (2005).
12:39PM W34.00008 Tuning of the critical current of superconducting nanowires by application of voltage pulses, THOMAS AREF, ALEXEY BEZRYADIN, UIUC — The critical current of superconducting nanowires may depend on a number of factors such as dimensions of the nanowire, the wire’s normal resistance or the presence of magnetic impurities. Determining which factors are most important is key to developing a detailed understanding of the underlying physics of 1D superconductivity. It is experimentally difficult to alter and probe such properties in situ at cryogenic temperatures. We have developed a method for tuning the critical current of a nanowire in situ inside a helium cryostat by the application of short, high bias voltage pulses. These pulses alter the critical current of the nanowire in a controlled manner by annealing or electromigration. Thus, for a single nanowire, we can vary critical current and normal resistance in situ. This process may have applications in developing future superconducting nanowire circuitry such as qubits where precise control of the nanowire’s critical current is required. We also discuss the dependence of the critical current on the normal resistance of the wire and compare to existing theories.

12:51PM W34.00009 Flux-quantization effect in superconducting niobium loops1, SUHONG YU*, ZHILI XIAO*, ALEXANDRA IMRE, JIONG HUA*, ULRICH WELP, WAI-KWONG KWOK, Argonne National Lab, Northern Illinois University — Superconducting loops have periodic oscillation of critical temperature $T_c$ as a function of applied perpendicular magnetic field $H$. The corresponding periodicity is related to superconducting flux quantization, $h/2e$, due to size constraint. When the loop size shrinks, however, new phenomena can appear. For example, the oscillation can show a $h/e$ rather than $h/2e$ periodicity if the hole diameter is comparable to the superconducting coherence length. We present experimental investigation of flux-quantization effect in mesoscopic superconducting niobium loops. We developed a new approach to fabricate high quality loops by combining electron-beam lithography with focused-ion-beam (FIB) milling techniques. Periodic oscillations were observed in both the $H - T$ phase diagram and the magnetoresistance. Analysis of the data with various theories will be presented.

1:03PM W34.00010 Anisotropic magnetoresistance of a one-dimensional superconducting niobium strip1, JIONG HUA*, ZHILI XIAO*, ALEXANDRA IMRE, SUHONG YU*, UMESH PATEL*, LEO OCOLA, RALU DIVAN, ALEXEI KOSELEV, JOHN PEARSON, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory, Northern Illinois University — We investigated confinement effects on the resistive anisotropy of a superconducting niobium strip with a rectangular cross-section. When the strip’s transverse dimensions are comparable to the superconducting coherence length, we find the angle dependent magnetoresistances at a fixed temperature can be scaled as $R(\theta, H) = R(H/H_{c1})$, where $H_{c1} = H_{c1}(\cos^2\theta - \sin^2\theta)^{1/2}$ is the angular dependent critical field, $\gamma = w/d$ is the width to thickness ratio of the strip, and $H_{c1}$ is the out-plane critical field at $\theta = 0$. Our results can be understood in terms of the anisotropic diamagnetic energy of a one-dimensional superconductor in a magnetic field.

1:15PM W34.00011 Quasi-reentrant resistive behavior in Bi$_2$Sr$_2$CaCu$_2$O$_8$ whiskers1, SEVDA AVCI, Northern Illinois University, UMESH PATEL, SUHONG YU, Argonne National Laboratory, Northern Illinois University, ZHILI XIAO, RALU DIVAN, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory, MILIND KUNCHUR, University of South Carolina — BSCCO (2212) whiskers were fabricated via a melt-quench-growth method and their morphology was characterized with scanning/transmission electron microscopy and atomic force microscopy. Four-probe magneto-transport measurements were conducted as a function of temperature and current. In low magnetic fields and currents, the resistance decreases monotonically and vanishes at a temperature of $\sim 80$ K. However, at large currents and magnetic fields the resistance shows a non-monotonic dependence on temperature, even showing values that are higher than the normal state resistance for certain ranges of the parameters. We attribute the observed behavior to the brick-wall morphology of the whiskers leading to a competition between normal and superconductive tunnelings that is known to take place in granular superconductive systems.

1:27PM W34.00012 Quenching of Meissner Diamagnetism in Superconducting Nanocrystals, HELENA MOREIRA, IRENE RESA, BENOT MAHLER, BENOT DUBERTRET, HERVE AUBIN, CNRS — We developed a new chemical synthesis for the preparation of high quality monodisperse superconducting Lead (Pb) nanocrystals. They are obtained from the alcohol reduction of Lead carboxylates in a hot organic solution and lead to colloids stabilized and protected from oxidation by organic ligands. Large quantities of nanocrystals with tunable diameter (8 to 30 nm) can be obtained. This new method allows the study of the effects of quantum confinement on superfluid response with unprecedented size resolution. Magnetic susceptibility measurements show that the large critical field of the particles increases from 2 to 5 T as the diameter is reduced down to 16 nm. This critical field results from the competition between the kinetic energy for Cooper pairs and superfluid condensation energy. Below the diameter of 16 nm, no Meissner effect remains in the particles, but only the signature of residual superconducting fluctuations. Remarkably the size scale below which the superfluid response disappears (16 nm) is significantly larger than the value expected from Anderson criterion. This implies that, in the regime of quantum confinement, there are distinct size-scales for the formation of Cooper pairs and the establishment of the superfluid response.

1:39PM W34.00013 Thin Superconducting Rings and Cylinders in a Magnetic Field, ROBERT BEAIRD, DANIEL E. SHEEHY, ILYA VEKHTER, Louisiana State University — We examine the magnetic field dependence of the critical temperature ($T_c$) for a thin superconducting ring and thin-walled superconducting cylinder (of radius $R$), in the presence of a magnetic field ($B$). We include both the orbital effect and the Zeeman splitting of the quasiparticle state. We derive a Ginzburg-Landau free energy functional and allow for the appearance of the spatially-modulated (Fulde-Ferrell-Larkin- Ovchinnikov) state. We explore the competition between the orbital effect and Zeeman splitting as a function of the ratio of $R$ to the superconducting coherence length, the orientation of $B$ with respect to the plane of the ring, and the Maki parameter (the ratio of the orbital and paramagnetic critical fields). We focus on the interplay of the periodicity and the overall suppression of $T_c$ with applied $B$.

1:51PM W34.00014 Order and Creep in Flux Lattices and CDWs Pinned by Planar Defects, ALEKSANDRA PETKOVIC, THOMAS NATTERMANN, Institute of Theoretical Physics, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany — The influence of randomly distributed point impurities and planar defects on the order and transport in type-II superconductors and related systems is considered theoretically. For random planar defects of identical orientation the flux line lattice exhibits a new glassy phase with diverging shear and tilt modulus, a transverse Meissner effect, large sample to sample fluctuations of longitudinal magnetic susceptibility and an exponential decay of translational long range order. The flux creep resistivity for currents $J$ parallel to the defects is $\rho(J) \sim \exp(-(J_0/J)^{\mu}$ with $\mu = 3/2$. Strong disorder enforces an array of dislocations to relax shear strain.
have recently observed phonon spectral anomalies in Nb and Pb that correspond to Kohn anomalies in the Fermi surface, at energies matching the low T conducting layered cuprates. The pairing of oxygen holes into heavy bipolarons in the paramagnetic phase (current-carrier density collapse (CCDC)) explains edge, but propagate as the Bloch states above the mobility edge. I identify the Froehlich EPI as the most essential for pairing and phase separation in super-

Attractive electron correlations, caused by an almost unretarded EPI, are sufficient to overcome the direct inter-site Coulomb repulsion in these charge-transfer and phase separation in the Hubbard model with on-site repulsive electron-electron correlations. I argue that microscopic phase separations in cuprate super-
critical exponents in terms of the inter-chain couplings and interaction parameters of the model.

This is particularly relevant for stripe phases in High Temperature Superconductivity arising from the Josephson tunneling between neighboring stripes, and is essentially a problem of dimensional crossover. Using inter-chain Mean Field Theory, we present results for the gaps, critical temperatures, and couplings. This is particularly relevant for stripe phases in High Temperature Superconductivity arising from the Josephson tunneling between neighboring stripes, and is essentially a problem of dimensional crossover. Using inter-chain Mean Field Theory, we present results for the gaps, critical temperatures, and critical exponents in terms of the inter-chain couplings and interaction parameters of the model.

We consider the problem of competing orders in a stripe phase with a large spin gap. In developing the phase diagram, we discuss the phases arising from the stabilization of the Superconducting (SC) and Charge Density Wave (CDW) orders by inter-stripe couplings. This is particularly relevant for stripe phases in High Temperature Superconductivity arising from the Josephson tunneling between neighboring stripes, and is essentially a problem of dimensional crossover. Using inter-chain Mean Field Theory, we present results for the gaps, critical temperatures, and critical exponents in terms of the inter-chain couplings and interaction parameters of the model.

Coherent Lattice Vibrations, Kohn Anomalies, and Pseudogaps in Superconductors

ALAN M. KADIN, Princeton Junction, NJ — A recent analysis has proposed [1] that the superconducting state is associated with charge density standing waves at k=2k_F, coupled to coherent lattice vibrations at 2k_F-G, where G is a reciprocal lattice vector. Independently, Aynajian et al. [2] have recently observed phonon spectral anomalies in Nb and Pb that correspond to Kohn anomalies in the Fermi surface, at energies matching the low T energy gap 2\Delta(0). Since Kohn anomalies are also defined by k=2k_F-G, these observations appear consistent with [1]. This also suggests that Kohn anomalies and an associated pseudogap provide a universal precursor of the superconducting state. Further experiments are proposed that should provide direct evidence of the coherent lattice vibrations in the superconducting state of conventional electron-phonon superconductors, and of alternative coherent oscillations (spin waves, etc.) in unconventional materials.


Crossed Andreev reflection dominated subgap transport in normal metal/superconducting hybrid structures

ANDREAS KLEINE, ANDREAS BAUMGARTNER, JELENA TRBOVIC, CHRISTIAN SCHONENBERGER, Department of Physics, Univ. of Basel, NANOELECTRONICS GROUP AT BASEL TEAM — We report on a systematic study of the non-local Andreev process (also called cross Andreev reflection = CAR) in planar mesoscopic N-S devices that consist of a superconducting (S) Al wire with several normal metal (N) fingers contacting the superconductor via tunneling barriers. We measure the non-local voltage appearing at a N (detector) contact located outside the current path, while a bias current is driven from another N (injector) contact to the S wire. This non-local differential signal has been studied as a function of bias and temperature for several samples with different N-S contact transparencies. In addition to CAR, elastic co-tunneling (EC) and charge imbalance (CI) appears in the measurements. We observe a systematic dependence of the relative magnitude of CAR, EC and CI. Most strikingly, CAR can dominate the subgap transport for all energies below the superconducting gap for a certain kind of sample. If the tunneling resistance R_t is increased, EC starts to dominate over CAR. This contribution is limited to small subgap biases, whereas CAR remains dominating at higher subgap biases. This dependence is explained by Coulomb blockade that becomes more prominent for increasing R_t.


11:15AM W35.00001 Gap anisotropy and universal pairing scale in a spin fluctuation model for cuprates

ARTEM ABANOV, Texas A&M University, ANDREY CHUBUKOV, University of Wisconsin, MICHAEL NORMAN, Argonne National Laboratory — We consider the evolution of \Delta_{z,y,z} pairing, mediated by nearly critical spin fluctuations, with the coupling strength. We show that the onset temperature for pairing, T^\ast, smoothly evolves between weak and strong coupling, passing through a broad maximum at intermediate coupling. At strong coupling, T^\ast is of the order of the magnetic exchange energy J. We argue that for all couplings, pairing is confined to the vicinity of the Fermi surface. We also find that thermal spin fluctuations only modestly reduce T^\ast, even at criticality, but they substantially smooth the gap anisotropy. The latter evolves with coupling, being the largest at weak coupling.

11:27AM W35.00002 Magneto-oscillations in Underdoped Cuprates

CHANDRA VARMA, University of California, Riverside — The conventional interpretation of the recent magneto-oscillation experiments in underdoped Cuprates, requires that there be a state of altered translational symmetry in the pseudogap state which is not supported by structural and Angle Resolved Photoemission Spectroscopy (ARPES) experiments. I show that the observed oscillations may be reconciled with the conclusion arrived in ARPES experiments that the fermi-surface, suitably defined, has the shape of four arcs which shrink to four points as the temperature T approaches 0. Experiments, including infrared absorption in a magnetic field, are suggested to distinguish between such a state obtained by the conventional interpretation of the magneto-oscillations.

11:39AM W35.00003 Phase Diagrams for Stripe Phases with a Spin gap

AKBAR JAEFARI, SIDDHARTHA LAL, EDUARDO FRADKIN, University of Illinois — We consider the problem of competing orders in a stripe phase with a large spin gap. In developing the phase diagram, we discuss the phases arising from the stabilization of the Superconducting (SC) and Charge Density Wave (CDW) orders by inter-stripe couplings. This is particularly relevant for stripe phases in High Temperature Superconductivity arising from the Josephson tunneling between neighboring stripes, and is essentially a problem of dimensional crossover. Using inter-chain Mean Field Theory, we present results for the gaps, critical temperatures, and critical exponents in terms of the inter-chain couplings and interaction parameters of the model.

11:51AM W35.00004 Phase separation of electrons strongly coupled with phonons in cuprates and manganites

SASHA ALEXANDROV, Loughborough University — Recent advanced Monte Carlo simulations have not found superconductivity and phase separation in the Hubbard model with on-site repulsive electron-electron correlations. I argue that microscopic phase separations in cuprate superconductors and colossal magneto-resistance (CMR) manganites originate from a strong electron-phonon interaction (EPI) combined with unavoidable disorder. Attractive electron correlations, caused by an almost unretarded EPI, are sufficient to overcome the direct inter-site Coulomb repulsion in these charge-transfer Mott-Hubbard insulators, so that low energy physics is that of small polarons and small bipolarons. They form clusters localized by disorder below the mobility edge, but propagate as the Bloch states above the mobility edge. I identify the Froehlich EPI as the most essential for pairing and phase separation in superconducting layered cuprates. The pairing of oxygen holes into heavy bipolarons in the paramagnetic phase (current-carrier density collapse (CCDC)) explains also CMR and high and low-resistance phase coexistence near the ferromagnetic transition of doped manganites.

12:03PM W35.00005 Coherent Lattice Vibrations, Kohn Anomalies, and Pseudogaps in Superconductors

ALAN M. KADIN, Princeton Junction, NJ — A recent analysis has proposed [1] that the superconducting state is associated with charge density standing waves at k=2k_F, coupled to coherent lattice vibrations at 2k_F-G, where G is a reciprocal lattice vector. Independently, Aynajian et al. [2] have recently observed phonon spectral anomalies in Nb and Pb that correspond to Kohn anomalies in the Fermi surface, at energies matching the low T energy gap 2\Delta(0). Since Kohn anomalies are also defined by k=2k_F-G, these observations appear consistent with [1]. This also suggests that Kohn anomalies and an associated pseudogap provide a universal precursor of the superconducting state. Further experiments are proposed that should provide direct evidence of the coherent lattice vibrations in the superconducting state of conventional electron-phonon superconductors, and of alternative coherent oscillations (spin waves, etc.) in unconventional materials.


12:15PM W35.00006 Phase-fluctuations model for the pseudogap of high temperature superconductors

WONKEE KIM, YAN CHEN, C. S. TING — Within the phase fluctuation picture for the pseudogap state of a high-T_c superconductor, we incorporate the phase fluctuations generated by the classical XY model with the Bogoliubov-de Gennes formalism utilizing a field-theoretical method. This picture delineates the essential characteristics of spatially varying local order parameters observed in high-T_c superconductors above T_c. We also compute the local density of states near a non-magnetic impurity with a strong scattering potential. The resonance peak smoothly evolves as temperature increases through T_c without showing any sudden broadening, which is consistent with recent experimental findings.
12:27PM W35.00007 Antiferromagnetic to singlet transition in the quarter-filled band. R.T. CLAY, Mississippi State University, S. MAZUMDAR, University of Arizona — One of the greatest challenges in constructing a theory of superconductivity in the presence of strong electron-electron (e-e) interactions is to describe how a transition can occur from antiferromagnetic to singlet order. Transitions between antiferromagnetism (AFM) and singlet order are well known in several specific cases such as the spin-Peierls (SP) transition, dimerization in the presence of antiferromagnetic nearest neighbor and second neighbor couplings, and the nongapped singlet in the rectangular spin ladder. In all three examples, the transition is a consequence of confinement within a quasi-one-dimensional lattice. Similar AFM/singlet transitions have not been found in the two dimensional (2D) 1/2-filled band. We present evidence that an AFM/singlet transition can occur in a 2D 1/4-filled anisotropic triangular lattice. A key difference is that at 1/4 filling, inhomogeneity in the form of coexisting charge, bond, and spin orders occur due to e-e and electron-phonon interactions. We show that with increasing lattice frustration the ground state of the 1/4-filled band anisotropic triangular lattice changes from AFM to a charge-ordered state with local singlets. Our results have direct implications for the 1/4-filled organic superconductors as well as related inorganic materials such as Na$_2$CoO$_2$, LiTi$_2$O$_4$, CuRh$_2$S$_4$. Supported by DOE grant DE-FG02-06ER46315.

12:39PM W35.00008 Collective Fluctuations of the Loop-Current Phase in Cuprates, ARKADY SHEKHTER, VIVEK AJI, CHANDRA VARMA, UC Riverside — We have calculated the collective modes of the loop-current ordered phase observed in underdoped Cuprates. Besides the modes given by the fluctuations of the Ashkin- Teller model, we find that the current fluctuations introduce a mode whose properties are similar to that of electro-magnetic vector potentials. We calculate the coupling of such a mode to the Ashkin-Teller modes and to the Fermions. 

12:51PM W35.00009 Superconductivity in Spin-Chain Ladder Cuprate, SHIGERU KOIKEGAMI, Second Lab, LLC, TAKASHI YANAGISAWA, Nanoelectronics Research Institute, AIST — We study the superconductivity in the three-dimensional d-p model with the quasi-one-dimensional structure in which CuO$_2$-chain and Cu$_2$O$_2$-ladder are alternately stacked with each other. When we control the hole density on each Cu site in our model, we have two or three Fermi surfaces, on which the fully-gapped superconductivity develops. Both the inter-band nesting and the large density of states around Van Hove singularity points play essential roles to achieve the superconductivity, and these two factors can coexist easily owing to the electron transfer between chain and ladder.

1:03PM W35.00010 Superconducting Fluctuations in Strongly Correlated Electronic Systems, WILLIAM PUTIKKA, Physics Department, Ohio State University — Superfluid behavior is relatively common in strongly correlated fermion systems. This suggests there is a common reason for this behavior rooted in the strong correlations. I propose such a mechanism, developed in the context of the 2D t-J model, where $d_{x^2-y^2}$ superconducting fluctuations have recently been observed. The $d_{x^2-y^2}$ fluctuations are not due to antiferromagnetic fluctuations; the AF fluctuations compete with superconducting fluctuations. Pair fluctuations have their own, separate origin based in the strong correlations. If the on site repulsion is strong enough it can affect the electronic degrees of freedom while the entropy still dominates the free energy. This requires the entropy to be maximized under the constraint of no double occupancy, thereby rearranging the electronic degrees of freedom into separate spin and charge excitations. These excitations have different statistics and very different energy scales, allowing the charges to develop pair correlations before the spin degrees of freedom become coherent. Below the spin coherence temperature, the spins determine the symmetry of the pair wave function for the electronic pair fluctuations. The symmetry which best avoids the AF fluctuations on a square lattice is $d_{x^2-y^2}$.


1:15PM W35.00011 The quantum effective potential and the condensation of topological excitations in Josephson junction arrays, SAID SAKHI, College of Arts and Sciences, American University of Sharjah, PO Box 26666, Sharjah, UAE — I analyze the radiative corrections to the effective potential for an Abelian gauge theory relevant to Josephson junction arrays (JJA). This model consists of two disorder fields related to electric and magnetic charges coupled to topologically gauge fields described by Maxwell terms and a mixed Chern-Simons term. The symmetry of the ground state is studied through the effective potential which takes into account radiative corrections in the theory. Here zero condensation for the topological charge excitations describe [1] insulating phases of JJA, and nonzero condensates describe superconducting phases. The gauge fields contribution to the one-loop effective potential is evaluated and its effect on the spontaneous symmetry breaking is examined. Effects of dissipation driving coupling in JJA systems connected to a reservoir of gapless single-particle excitations are also studied. Coupling to gapless fermions is shown to induce radiative corrections in the effective potential which favor transitions between an insulating state and a superconducting state. [1] S. Sakh, Europhys. Lett. 73 (2), 267 (2006).

1:27PM W35.00012 Topological Confinement and Superconductivity, KHALED AL-HASSANIEH, CRISTIAN BATISTA, PINAKI SENGUPTA, Los Alamos National Laboratory, ADRIAN FEIGUIN, University of Maryland — We derive a Kondo Lattice model with a correlated conduction band from a two-band Hubbard Hamiltonian. This mapping allows us to describe the emergence of a robust pairing mechanism in a model that only contains repulsive interactions. The mechanism is due to topological confinement and results from the interplay between antiferromagnetism and delocalization. By using Density-Matrix-Renormalization Group (DMRG) we demonstrate that this mechanism leads to dominant superconducting correlations in a 1D-system. [1] K.A. Al-Hassanieh, C. Batista, P. Sengupta, and A. E. Feiguin, preprint arXiv:0808.3735.

1LANL is supported by the U.S. DOE under Contract No. W-7405-ENG-36.

1:39PM W35.00013 Vortex lattice structures of spin triplet superconductors, DANIEL AGTERBERG, University of Wisconsin - Milwaukee, SUK BUM CHUNG, Stanford University, EUN-AH KIM, Cornell University — Motivated by recent interest in spin triplet superconductors, we investigate the vortex lattice structures for this class of unconventional superconductors. We discuss how the order parameter symmetry can give rise to $U(1) \times U(1)$ symmetry in same sense as in spinor condensates, making the half-quantum vortex (1/2-qv) topologically stable. We then calculate the vortex lattice structure of 1/2-qv’s, with particular attention on the roles of the crystalline lattice, the Zeeman coupling, and Meissner screening, all absent in spinor condensates. Finally, we consider how spin-orbit coupling leads to a breakdown of the $U(1) \times U(1)$ symmetry and the fate of the 1/2-qv lattice. As examples, we consider models for spin-triplet superconductivity in Sr$_2$RuO$_4$ and more speculative spin-triplet models for Na$_2$CoO$_2$·yH$_2$O and Bechgaard salts.

1:51PM W35.00014 Strong coupling limit of superconductivity in anti-ferromagnetic phase: Extended hardcore boson picture of d-wave order and phase fluctuation, YUCEL YILDIRIM, WEI KU, Brookhaven National Laboratory — Strong coupling limit (local-pairing >> kinetic energy) of the superconductivity in High-Tc superconductors is investigated within the anti-ferromagnetic phase. An extended hardcore boson picture consisting of paired holes results from general considerations of paired fermions, in which directional near-neighbor occupations of bosons are forbidden. By use of Wannier function of the low-energy sector of the bosonic Hilbert space, our simple picture provides a natural separation of the phase of the superconducting order parameter into local and external ones. Within a realistic parameter range, the local structure is found to be of d-wave symmetry, driven by the kinetic energy. On the other hand, the genuine behavior of the superconductivity is controlled by the phase coherence of the external phase, which leads to experimentally observed linear reduction of super fluid density. Interestingly, due to the competition with p-wave symmetry, the effective mass of the boson is enormously enhanced from that of the Fermion, explaining the very small stiffness. Connections to recent observation of 4-period d-wave CDW in the "stripe" phase, and C2-symmetry bond-centered charge profile will also be addressed.
2:03PM W35.00015 A new method for solving the inhomogeneous Bogoliubov - de Gennes equations. LUCIAN COAVACI, MONA BERCIU, University of British Columbia, Vancouver, Canada — Inhomogeneities (surface, interfaces, impurities, etc.) in superconductors give rise to interesting phenomena, like broken time-reversal states, bound states near surfaces, etc. Numerical solutions of the self-consistent Bogoliubov-de Gennes mean field equations become computationally intensive for systems whose translational symmetry is broken. We propose a new method of solving the mean-field equations based on the Kernel Polynomial Method. We expand the Green’s functions in terms of Chebyshev polynomials and calculate the order parameters self-consistently. Because the most expensive operation is only the sparse matrix-vector multiplication, the benefits of this method are multiple: usage of large systems, easy implementation of symmetries, multiple bands. Although we apply this method to a specific example (formation of Andreev states in 2D superconductors), it is applicable to any mean-field calculation.


11:15AM W36.00001 Conductance of a fully equilibrated quantum wire1, TOBIAS MICKLITZ, JEROME RECH, K. A. MATVEEV, Argonne National Laboratory — We study electronic transport properties of a long weakly interacting homogeneous quantum wire, connected to non-interacting leads. From Galilean invariance of the system we infer that in a state with a finite electric current, the electrons reach thermal equilibrium in a frame moving with their drift velocity. At non-zero temperature the resulting distribution function inside the wire is slightly different from the distribution supplied by the leads. This gives rise to a small correction to the quantized value of conductance 2e2/h, which can be found by performing a careful analysis of the conservation laws. The correction is of the order of (∂E_F/∂T)^2 and does not depend on the details of the electron-electron interaction.

1This work is supported by the US DOE, Office of Science, under Contract No. DE-AC02-06CH11357

11:27AM W36.00002 Simulation of electron conduction in a prototypical three-terminal molecular transistor. HAIYING HE, RAVINDRA PANDEY, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRD-ARL-WM; Aberdeen Proving Ground, MD 21005-5069 — In a single molecule, electronic charge can be modulated either by electrical field or by chemical effects, thereby opening up the possibility of their use as active elements in electronic devices. In this talk, we present the results of a theoretical study on the electronic conduction of a novel, three-terminal molecular architecture, analogous to a heterojunction bipolar transistor. In this architecture, two diode arms consisting of donor-acceptor molecular wires fuse through a ring, while a gate modulating wire is a π-conjugated wire. The calculated results show the enhancement or depletion mode of a transistor by applying a gate field along the positive or negative direction. A small gate field is required to switch on the current in the proposed architecture. The changes in the electronic conduction can be attributed to the intrinsic dipolar molecular architecture in terms of the evolution of molecular wavefunctions, specifically the one associated with the terphenyl group of the modulating wire in the presence of the gate field.

11:39AM W36.00003 Synthesis and metal-to-semiconductor conversion of carbon nanotubes by light irradiation. LEWIS GOMEZ DE ARCO, AKSHAY KUMAR, YI ZHANG, KOUNGMIN RYU, ALEXANDER BADMAEV, CHONGWU ZHOU, Electrical Engineering - University of Southern California — We report on the synthesis of aligned nanotubes on Sapphire and quartz substrates, transfer, device fabrication and scalable light-to-semiconductor conversion of carbon nanotubes on field-effect transistor (CNTFET) channels by broadband light irradiation at environmental conditions. Inactivation of metallic nanotubes in the channels was achieved as a consequence of a light-assisted photochemical process that led to a controlled sp^2 to sp^3 transition in the nanotubes structure, and hence localization of π-electrons. Stronger gate bias dependence with improvements in the drain current On/Off ratio up to 10^5 was found in around 90 percent of the CNTFETs. The possibility of fabricating mostly semiconducting carbon nanotube transistors by simple light irradiation in air over entire wafers constitutes an important achievement in terms of assembly, integration and large scale fabrication of nanotube-based circuits.

11:51AM W36.00004 Spectroscopic and structural studies of L-arginine doped Potassium Dihydrogen Phosphate crystals3. JAYESH GOVANI, CRISTIAN BOTEZ, WILLIAM DURRER, FELICIA MANCIU, Physics Department, University of Texas at El Paso, TX 79968 — We report in this study the spectroscopic and structural characterization of standard and L-arginine doped potassium dihydrogen phosphate crystals synthesized by a solution growth technique. The infrared absorption and Raman results demonstrate chemical functionalization between the amino (NH叁) groups of the organic material and the phosphate units of the inorganic crystals. This affirmation, which also implies the achievement of successful doping, is supported by the existence of extra vibrational lines in the IR and Raman spectra of L-arginine doped potassium dihydrogen phosphate crystals; these vibrational lines exhibit shifting towards lower frequencies as compared with the characteristic bands of L-arginine. Incorporation of the amino acid into the structure of the inorganic material is revealed by X-ray diffraction results also, where the shifting of diffraction lines and the appearance of a new one are observed.

3This work was supported by the NSF-MRI grant # 0723115. The authors are thankful to Dr. Mihir Joshi from Saurashtra University, Rajkot 360005, India, for providing the samples.

12:03PM W36.00005 Heteroborane Analogs of Silicon clusters: Experimental and Theoretical Studies on Bi2Si14. KIRAN BOGGAVARAPU, McNeese State University, MILEY JACKSON, McNeese State University, XING LI, ANDREJ GRUBISIC, DI WANG, KIT BOWEN, Johns Hopkins University, ANIL KANDALAM, McNeese State University, HAO-PENG WANG, Johns Hopkins University — Despite numerous studies, silicon clusters continue to fascinate. Part of the intrigue comes from the fact that, unlike metallic clusters which have strongly delocalized electrons and prefer to follow simple electron counting rules such as those originating from Jellium models, there are no simple rules of thumb that can be used to understand the diverse structures of silicon clusters. However, over the last couple of decades, there have been attempts to connect the structure and bonding of silicon clusters to a large class of well-studied three dimensional boron hydride compounds, specifically boranes, BnHn叁. By equating the π-lone pair of divalent silicon to a B-H bond, it was shown that the frontier orbitals of both units are similar. Theoretical studies have concluded that the silicon clusters (Si2nmin) adopt similar structural patterns to those of boranes, when n = 5, 6, 7, 8, 10 and 13. The question then arises, whether neutral analogs of Si2nmin and neutral heteroboranes, X2Bi2BnHn (X = N, P, Sb, Bi), can be envisioned. Here, we present the scope and limitation such analogy based on our recent theoretical (DFT) and experimental (anion-photoelectron spectroscopy) studies on Bi2Si14 (n = 4-8). In particular, we show that both Bi2Si14 and Bi2Si18 adopt similar pentagonal bipyramidal (PBP) geometries and have analogous orbital energy patterns.
12:15PM W36.00006 In situ characterization of crystal structure and physical properties of individual nanostructures in as-fabricated devices. MARCEL LUCAS, School of Physics, Georgia Institute of Technology, ZHONG LIN WANG, School of Materials Science and Engineering, Georgia Institute of Technology, ELISA RIEDO, School of Physics, Georgia Institute of Technology — Nanostructures have potential applications as electronic components, catalysts, sensors, biomarkers, and energy harvesters. Control over their morphology and structure is essential, since their physical properties depend on their dimensions and crystallographic structure. Although in situ transmission electron microscopy can correlate the structure and physical properties of individual one-dimensional nanostructures, it usually damages the sample and is unable to recover the characterized nanostructure for next-step device fabrication and application. Here, we demonstrate a method combining atomic force microscopy and polarized Raman spectroscopy to characterize in situ the morphology, crystal structure and physical properties of individual nanostructures that can be as-fabricated devices without sample damage. Based on scanning probe microscopy, our method can be extended to study the electronic, mechanical, and tribological properties of inorganic/biological nanostructures.

1Work supported by DOE under Grant No. DE-FG02-06ER42993 and NSF.

12:27PM W36.00007 Simulating self-assembly of porphyrin nanorods. GREGORY K. GUTHE, ADAM V. SUBHAS, WALTER F. SMITH, JOSHUA SCHRIER, Haverford College — Diadid meso-tetra(4-sulfonatophenyl)porphine (TPPS4−) monomers have been shown to self assemble into nanorods with well-defined cross-section and intriguing photoelectronic properties. However, the structure and conduction mechanism of these nanorods is poorly understood, and questions remain about the aggregation process. Using density functional theory (DFT), we first obtain optimized geometries and atomic-charges for the monomers, which we then use for subsequent molecular dynamics (MD) simulations to observe the initial stages of the self-assembly process. This work uses the resources of the National Energy Research Scientific Computing Center. A.D. Schwab et al., J. Phys. Chem. B 107, 11339 (2003). A.D. Schwab et al., Nano Letters 4, 1261 (2004).

12:39PM W36.00008 Electric field directed growth of cuprous oxide nanostructures for photon sensing. SANGEETA SAHOO, SAROJ NAYAK, Rensselaer Polytechnic Institute, PULICKEL AJAYAN, Rice University — We demonstrate an electro-deposition technique to synthesize cuprous oxide nanomaterials in various types of nanostructural form at room temperature. We apply an electric field under deionized water on the top electrode with the conductive substrate made of Cu. Using this method, direct growth of nanostructures has been achieved on different types of substrates. We show that the structural evolution depends strongly on the electric potential between the electrodes and also on the type of substrates. We have studied the growth mechanism on flat Si substrate and on Transmission electron Microscopy grid. A variety of structures from simple one dimensional nanowires to different complex two and three dimensional structures are successfully grown directly on substrates with this method. Direct integration of these nanostructures on substrates paves the way to step ahead towards the fabrication of electronic devices. Taken together, this novel technique of Cu2O nanostructure production is highly reproducible, catalysts free, fast and a low cost simple process. In addition, the electrical characteristics indicates the usefulness of these structures for photo-sensing and optoelectronic applications.

12:51PM W36.00009 Ca1+xCoB1 and Ca1+xRuB4: New Borides with One-Dimensional Channel Structures. YUKARI KATSURA, HIRAKU OGINO, YUTAKA MATSUMURA, Department of Applied Chemistry, the University of Tokyo, KAZUMASA SUGIYAMA, TOETSU SHISHIDO, Institute for Materials Research, Tohoku University, SHIGERU HORII, JUN-ICHI SHIMOYA, KOJI KISHIO, Department of Applied Chemistry, the University of Tokyo — We discovered two novel borides Ca1+xCoB1 (x = 0.10) and Ca1+xRuB4 (x = 0.18) as the first members of Gd1−xFe2B2−x and Pr1−xRe2B2−x-type ternary borides with a divalent metal at the rare earth sites. In these compounds, tetrahedral chains of transition metals and boron form tetradimensional channel structures, which contain single atomic chains of Ca. These are composed of CoB4 and RuB4 sublattices, with common a-axis lengths and independent c-axis lengths. The two structural types are distinguished by configurations of the tetrahedral chains. Resistivity and magnetization measurements showed that these compounds are paramagnetic metals down to 2 K. Preliminary first-principle calculations indicated the presence of covalent bonds between transition metals and boron, and electrical conductivity originating from the d-bands of the transition metals.

1:03PM W36.00010 Photoluminescence Studies of Hydrogenated a-Silicon Carbide. SOMILKUMAR RATHI, Colorado School of Mines, FENG ZHU, MVSystems,Golden,CO, JOSHUA GALLON, BRIAN SIMMONDS, GEORGE RADZISZEWSKI, P. CRAIG TAYLOR, Colorado School of Mines — A series of PECVD grown silicon carbide samples differing in their carbon content was investigated by a near-IR FT-Photoluminescence (PL) technique. The goal of this study was to establish a correlation between carbon concentration in a-SiC and the observed luminescence signal. Variations in the observed temperature dependences of the PL signals in a-SiC are attributed to differences in the carbon content. The samples, initially kept at 18 K on a closed-cycle helium cryostat, were excited with Ar-ion laser light at 514.5 nm (with power ranging 5-30 mW; and a flume of 0.5 to 3 W/cm2), and the luminescence was recorded with an InGaAs detector over the range of 1.5 eV to 0.67 eV. There was no change in PL intensity below 50 K; above 50 K the intensity decayed logarithmically up to room temperature. The increase of carbon content caused an increase in the PL on the higher energy side of the emission peak (approximately centered at 1.29 eV; FWHM = 0.3 eV) with concurrent intensity decrease on the lower energy side.

1This research is partially supported by NSF and REMRSEC.

1:15PM W36.00011 Electrical transport in YSi2 nanowires. V. IANCU, Department of Physics, University of Tennessee, P.R.C. KENT, T.-H. KIM, A.-P. LI, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, L.D. MENARD, J.M. RAMSEY, Department of Chemistry, University of North Carolina, Chapel Hill, H.H. WEITERING, University of Tennessee — When a small amount of yttrium is deposited onto Si, silicon islands in ultrathin films form. In subsequent metal deposition, the yttrium atoms self-assemble into highly uniform silicide nanowires with dimensions of the order of 4x1.1x1000 nm3. These YSi2 nanowires are among the thinnest silicide structures fabricated to date. Their electrical properties have been explored using a four-probe scanning tunneling microscope (STM). The wires exhibit ohmic conduction at room temperature but the conductance decreases at lower temperature. STS measurements [1] indicated a small gap opening at low temperature in the thinnest YSi2 wires, which appears to be associated with the charge-order fluctuations seen in STM. The YSi2 nanowires not only represent an interesting model system for exploring 1D quantum transport, but they can also be used as electronic/multicomponents in nanoscale electronic devices on silicon substrates. The research at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences was sponsored by the National User Facilities Division, U.S. DOE. [1] C. Zeng et al. Nat. Mat. 7, 539 (2008)

1:27PM W36.00012 Gate-tunable magnetic exchange and giant g-factor fluctuations in InAs nanowire quantum dots. SZABOLCS CSONKA, LUKAS HOFSTETTER, FRANK FREITAG, STEFAN OBERHOLZER, CHRISTIAN SCHONENBERGER, Department of Physics, Univ. of Basel, THOMAS SAND JEPSEN, MARTIN AGASEN, JESPER NYCARD, Niels Bohr Institute, Copenhagen, NANOELECTRONICS GROUP AT BASEL TEAM, NANOSCALE QUANTUM ELECTRONICS GROUP AT THE NANO-SCIENCE CENTER TEAM — We use the spin-1/2 Kondo effect, which is observed in every other charge ground state with odd elec-trons, to measure the field-induced splitting of the spin-doublet, and hence the g-factor. We do this in hybrid quantum dots using both normal (N), ferromagnetic (F) and superconducting (S) contacts. Unlike to previous studies, the g-factors of neighboring states can vary a lot: g can scatter between 2 and 18 and can therefore be even larger than in the bulk (g ~ 15). We demonstrate further the electric gate tunability of the g-factor in a single charge state. When using F contacts, a zero-field splitting is induced. The proximity-induced exchange field has recently been measured for the first time by Hauptmann et al. (Nature Physics 4, (2008)) in carbon nanotubes. Here, we show the same effect in a semiconductor nanowire, demonstrating that this effect is universal. Employing a pair of S and F contacts, the proximity-induced exchange shows up as a minigap in superconducting spectroscopy.
There is a correlation between binding energy ($E_2$) and energy band gap ($E_g$) of TiO$_2$ nanowires. In general, $E_g$ increases with increasing $E_2$. In TiO$_2$ nanowires, both metallic and semiconductor nanowires are resulted. In this case, in addition to paramagnetic TiO$_2$ nanowires, there are also ferromagnetic ones. We have also studied the structural and electronic properties of bulk-like rutile (110) nanowires. There is a crossover in terms of energetics and bulk-like nanowires are more stable than the thin nanowires for larger radius wires after a critical diameter. These (110) rutile nanowires are all semiconductors.

We start, by way of first-principles calculations, the existence of a giant nonlinear flexoelectric effect in BN 2D strips. The induced polarization is quadratic in amplitude of atomic displacements $A$, yet the dipole moment per unit cell is about four times larger compared to PbZrTiO$_3$ [1]. The new effect may find a variety of practical applications and, in particular, as nanogenerators and tactile sensors powered by an ambient motion or agitation. BN material is inert and can be used in biological environment.

We have systematically investigated structural, electronic and magnetic properties of very thin TiO$_n$ ($x$=1,2) nanowires as well as bulk-like (110) rutile nanowires by using the first principles plane wave pseudopotential calculations based on density functional theory. A large number of different possible structures have been searched via total energy calculations in order to find the ground state structures of these nanowires. Three dimensional structures have been searched for both of the stoichiometries (i.e. $x$=1,2). The stability of TiO$_n$ nanowires enhances with its increasing radius, thus reaching sufficient coordination number of Ti and O atoms. All stoichiometric TiO$_2$ nanowires studied exhibit semiconducting behavior and have nonmagnetic ground state. There is a correlation between binding energy ($E_b$) and energy band gap ($E_g$) of TiO$_2$ nanowires. In general, $E_b$ increases with increasing $E_g$.
12:27PM W37.00007 Application of the Finite-Element Space-Time Algorithm to Bound States$^1$, CHARLES WEATHERFORD, Florida A&M University, ALBERT WYNN, DANIEL GEBREMEDHIN, XINGJUN ZHANG, Florida A&M University — The implementation of the Dirac representation is facilitated by the finite element space-time algorithm.$^1$ Multicenter integral computations are also facilitated by this same algorithm. The present work is the first application of this original algorithm to the computation of bound states of atoms and molecules. The Dirac representation is employed such that $H_0$ is the sum of the one-electron operators while the residual $H_1$ is the sum of the two-electron operators. Soft-Coulombic geminals are then used as the basis for the time-dependent calculation of a superposition of the bound-states. The eigenstates and eigenvalues are then extracted by filter-diagonalization. An addition theorem is given for the soft-coulombic geminals and the geminals are translated again using the space-time algorithm, so that multicenter integrals may be computed. Several small atoms and molecules are considered as an illustration of the method.$^1$

$^1$Supported by the NSF CREST Center for Astrophysical Science and Technology.

12:39PM W37.00008 Test of Current Variational Procedures for Electronic Structures and Properties of Molecular and Solid State Systems by application to Atomic Systems$^1$-H$^-$ Ion, HARI PAUDEL, ARCHANA DUBEY, UCF Orlando, R.H. SCHEICHER, Uppsala University, Sweden, S.R. BADU, R.H. PINK, T.P. DAS, SUNY Albany — Electronic properties of atomic systems are obtainable using Linked Cluster Many-Body Perturbation Theory (LCMBPT) with high accuracy and excellent agreement with experiment, using complete sets of states obtained by differential equation procedures$^1,2$. Unfortunately such procedures are not practicable for multi-center molecular and solid state problems and variational procedures have to be used for obtaining the occupied and excited one electron states to work on electronic properties of the latter systems. With the aim to assess the accuracies of the latter procedures with Gaussian basis states, like the first principles Hartree-Fock procedure together with many body perturbation theory, and density functional based procedures, we are testing them for both energy and wave function dependent properties of atoms. Results will be presented for H$^-$ ion, where Hartree-Fock theory predicts instability with respect to auto ionization to H atom and electron correlation effects obtained by the LCMBPT procedure$^3$ restore stability, providing nearly exact experimental affinity for H$^-$.$^1$[1] Alfred Owusu et al., Phys. Rev. A56, 305(1997)$^2$[2] T.Lee et al., Phys. Rev. A4 1410(1971)$^3$[3]C.M. Dutta et al., Phys. Rev. A2, 2289(1970)

12:51PM W37.00009 Computation of Nonlinear Impedance Spectra in Samaria Doped Ceria$^1$, FRANCESCO CIUCCI, California Institute of Technology — Samarium Doped Ceria (SDC) electrodes are currently of great interest for solid oxide fuel cells (SOFC) applications. For example, ceria-containing anodes can be operated directly on hydrocarbons without coking, and in addition can be used at lower temperatures than Ni/YSZ. In order to design, optimize, and characterize electrodes, it is very useful to have models to aid in interpreting experimental results. In this work, we present a non-linear, time-dependent model for the study of SDC. This model allows us to compute species concentrations, electric potential and currents under medium bias conditions. A regular perturbation of the drift diffusion equations and Poisson’s equation is used to derive the model for the behavior of bulk of the material. We also include the kinetics of reactions occurring at the SDC-gas surface where the SDC is exposed to a spatially uniform hydrogen-water-argon mixture at fixed total pressure. The numerical procedure allows for fast computations and for the direct determination of fast and rate limiting steps. Impedance spectra are computed in the 2D case and a quantitative comparison between experimental (symmetric cell) and numerical results is presented. Our model can be naturally extended to the non-symmetric case, i.e. the case under which the two sides of the SDC assembly are exposed to different atmospheres.

1:03PM W37.00010 An Analytical Approach to Computing Biomolecular Electrostatic Potential$^1$, ANDREW FENLEY, JOHN GORDON, ALEXEY ONUFRIEV, Virginia Tech — Analytical approximations to fundamental equations of continuum electrostatics on simple shapes can lead to computationally inexpensive prescriptions for calculating electrostatic properties of realistic molecules. Here, we derive a closed form, analytical approximation to the Poisson equation for an arbitrary distribution of point charges and a spherical dielectric boundary. The simple, parameter-free formula defines continuous electrostatic potential everywhere in space and is obtained from the exact infinite series (Kirkwood) solution by an approximate summation method that avoids truncating the infinite series. We show that keeping all the terms proves critical for the accuracy of this approximation, which is fully controllable for the sphere. We apply the approximation to 580 biomolecules under realistic solvation conditions, where the effects of mobile ions are included at the Debye-Hückel level. The accuracy of the approximation as applied to the biomolecules is assessed through comparisons with numerical Poisson-Boltzmann (NPB) reference solutions. For each structure, the deviation from the reference is computed for a large number of test points placed near the dielectric boundary (molecular surface). The accuracy of the approximation is within 1 kT per unit charge for 91.5% of the individual test points.

1:15PM W37.00011 Ab initio Study of Atomic and Molecular Polarizabilities$^1$, IGOR VASILIEV, New Mexico State University, JAMES R. CHELIKOWSKY, The University of Texas at Austin — We calculate the static electric dipole polarizabilities for a variety of atoms and molecules using a finite field method implemented in the framework of an ab initio density functional formalism. Our calculations employ several different representations of the exchange-correlation potential, including the local density approximation, generalized gradient approximation, and asymptotically correct functionals introduced by Leeuwen-Baerends$^1$ and Casida-Salahub$^2$. We observe that the computed values of polarizabilities are strongly influenced by the asymptotic behavior of the density functional exchange-correlation potential. The accuracy of theoretical atomic and molecular polarizabilities is substantially improved by the use of asymptotically correct exchange-correlation functionals. This result can be explained in terms of electronic excitation energies and the polarizability sum rule.

$^1$This work was supported in part by NSF under DMR-0551195, ACS under PRF-48556-AC10, and the U.S. Department of Energy under DE-FG36-08GO88008, DE-FG02-06ER46286, and DE-FG02-06ER15760.

1:27PM W37.00012 Theoretical predictions of the impact of nuclear dynamics and environment on core-level spectra of organic molecules, DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, CRAIG SCHWARTZ, JANIEL UEJIO, RICHARD SAYKALLY, Chemical Sciences Division, Lawrence Berkeley National Laboratory — Core-level spectroscopy provides an element-specific probe of local electronic structure and bonding, but linking details of atomic structure to measured spectra relies heavily on accurate theoretical interpretation. We present first principles simulations of the x-ray absorption of a range of organic molecules both in isolation and aqueous solution, highlighting the spectral impact of internal nuclear motion as well as solvent interactions. Our approach uses density functional theory with explicit inclusion of the core-level excited state within a plane-wave supercell framework. Nuclear degrees of freedom are sampled using various molecular dynamics techniques. We indicate specific cases for molecules in their vibrational ground state at experimental conditions, where nuclear quantum effects must be included. Prepared by LBNL under Contract DE-AC02-05CH11231.
Efficient free energy calculations of quantum systems through computer simulations

Alex Antonelli, Universidade Estadual de Campinas, Rafael Ramirez, Carlos Herrero, Instituto de Ciencia de Materiales de Madrid, Eduardo Hernandez, Instituto de Ciencia de Materiales de Barcelona

In general, the classical limit is assumed in computer simulation calculations of free energy. This approximation, however, is not justifiable for a class of systems in which quantum contributions for the free energy cannot be neglected. The inclusion of quantum effects is important for the determination of reliable phase diagrams of these systems. In this work, we present a new methodology to compute the free energy of many-body quantum systems. This methodology results from the combination of the path integral formulation of statistical mechanics and efficient non-equilibrium methods to estimate free energy. Namely, the adiabatic switching and ensemble averaging methods. A quantum Einstein crystal is used as a model to show the accuracy and reliability the methodology. This new method is applied to the calculation of solid-liquid co-existence properties of neon. Our findings indicate that quantum contributions to properties such as, melting point, latent heat of fusion, entropy of fusion, and slope of melting line can be up to 10% of the calculated values using the classical approximation.

Applications of a novel QM/MM method incorporating a polarizable force field

Christopher Williams, John Herbert, Ohio State University

In conventional QM/MM methods the MM region is modeled by a force field that uses a set of point charges to represent the electrostatics. However, recently developed force fields use multipole expansions combined with polarizable sites to represent electrostatic interactions. A novel algorithm is presented to incorporate this class of force fields with a QM region by allowing the QM region and the MM region to share the same computational cell. This algorithm is implemented in the software package TINKER. The algorithm is general and can be used with a variety of QM methods including MP2 and DFT. Examples of both ground state and excited state calculations are presented, including the investigation of the effectiveness of many-body expansions in modeling the solvation of charged species and the effect of charged environments on biomolecules.

Numerical modeling of fast gate-coupled ion permeation in CIC channels

Mary H. Cheng, Department of Chemistry, University of Pittsburgh

We have developed a three dimensional Brownian dynamics (BD) and discrete-state model to couple ion permeation to the motion of a putative fast gate in the CIC channels. The model channel is designed so as to represent certain essential features of CIC chloride channel, in which a glutamate side chain moves from an open state to a closed state (blocking the channel pore at a position which also acts as a binding site for Cl	extsuperscript{−} ions moving through the channel). Both BD and the discrete-state model generate results in qualitative agreement with experimental observations and consistent with the foot-in-the-door mechanism. Furthermore, we have formulated a numerical approach to calculate the discrete rate constants in our model channel using BD. The discrete-state model with the rate constants solved via BD produces results consistent with the (continuous space) multi-ion BD simulations.

Modeling Ion Solvation and Transport through Chloride Transport Proteins

Thomas Beck, Univ. of Cincinnati

Ion channels and transporters are membrane proteins that selectively conduct ions either passively (channels) or actively using a chemical gradient of one ion (transporters). The H+/Cl	extsuperscript{−} transporter, first discovered in bacteria, has now been shown to also occur in animals and plants. This talk will discuss computational approaches aimed at understanding the ion transit pathways through the bacterial chloride transporter. A Monte Carlo method (TransPath) that uses the crystal structure as input and exhaustively searches the protein for open pore spaces and favorable electrostatic domains has been developed. The algorithm successfully predicted pathways for the motion of chloride ions and protons. In order to better understand the free energies along the predicted transport pathways, we have developed a new statistical mechanical approach for computing absolute solvation free energies in restricted environments based on a quasi-chemical approach. Anion free energy results employing the new method will be presented.

Snug-fit, fluctuations, and metal-ion hydration in the selectivity of potassium ion channels

Lawrence Pratt, Chemical and Biomolecular Engineering, Tulane University

On the basis of molecular simulation, an identification of a single dominating physical factor responsible for Na\textsuperscript{+}/K\textsuperscript{+} selectivity of the KcsA channel has been contentious. The potential distribution theorem and quasi-chemical theory cast new light on the factors responsible for Na\textsuperscript{+}/K\textsuperscript{+} selectivity. In that context, we argue that an alternative definite formulation of the molecular statistical thermodynamic problem can help in achieving a consensus view of selectivity. We summarize the necessary new theoretical ingredients and published numerical results in working toward that consensus view.

Conformation changes in the Glutamate receptor as studied by LRET

Vasanthi Jayaraman, University of Texas Health Science Center at Houston

Glutamate receptors are the primary mediators of excitatory neurotransmission in the mammalian central nervous system. Glutamate binding to an extracellular ligand binding domain initiates a series of conformational changes that results in the formation of cationic pathways in the channel. The potential distribution theorem and quasi-chemical theory cast new light on the factors responsible for Na\textsuperscript{+}/K\textsuperscript{+} selectivity. In that context, we argue that an alternative definite formulation of the molecular statistical thermodynamic problem can help in achieving a consensus view of selectivity. We summarize the necessary new theoretical ingredients and published numerical results in working toward that consensus view.

Electric and Molecular Characteristics of Ion Channels

Richard Desantis, APS

A galvanic cell’s electrolyte is an insulator. A conductive electrolyte would quickly discharge a dry cell’s voltage. Voltage-producing paths within an electrolyte can develop spontaneously. A voltage-producing path must bridge from the anode to the cathode, to export voltage out of the insulting electrolyte. Doubling cathode to anode distance does not decrease the cell’s fixed output voltage. The fixed voltage indicates superconductor-like behavior. Gaps between voltage-producing molecules would isolate the anode from the cathode, preventing superconductor-like behavior. Gating activity within membrane protein complexes can prevent or allow voltage-producing paths. A voltage-producing path is a single molecule containing both anode and cathode reactants. Only combined anode-cathode reactions within a single molecule can produce the cell’s fixed exterior voltage. While within the single molecule, atoms can relocate and react. In a lead acid cell, charging voltage raises the molecule’s energy state. The extra energy allows Pb and PbO2 to form during the molecule’s collapse. For discharging, an external circuit provides an outlet for the molecule’s voltage, which lowers the molecule’s energy state to a level that permits PbSO4 production.
that this lack of motion is not due to signal relay. Our results indicate that a quorum sensing mechanism exists which is closely coupled to chemotaxis.

of motion appears unaffected by the formation of streams. At large cell-cell distances cells do not form streams in response to externally applied chemical gradient. Analysis of cell tracks outside and within streams shows that cells do not speed up or slow down when moving as a group. In addition the persistence element in many biological processes, such as embryogenesis and cancer metastasis. The aim of our study is to quantify chemotaxis of groups of cells. We find

PARENT, National Cancer Institute, NIH, COLIN MCCANN, University of Maryland and NCI — Cell migration up an external chemical gradient is a crucial based on live cell-imaging (J Neurosci. 2007, 27:507, Mol Biol Cell. 2005, 16:4243). We use this model to predict changes in axonal morphology upon local

axonal caliber and as a result, the kinetics of NF movement determines the overall shape of the axon. We developed a kinetic model for movement of NFs at the average slow rate of \(0.5\text{ mm/day}\). Characterized by bursts of movement and extended pauses in between. The local number of NFs determines the local shape, as well as the locations and intensities of certain intracellular signals. We found that when cells undergoing chemokinesis, random migration in response to a chemical signal, are directed off of a cliff, they do not fall off the cliff. Instead, they search for new attachment points, eventually change direction, and continue moving along the edge of the cliff. Both ridges and cliffs affect more than just the motion of a cell; they also affect its shape.

Dictyostelium discoideum

of cellular migration, an important physiological process that occurs in embryonic development, wound healing, and cancer metastasis. We study the motion of \(D.\) discoideum on surfaces with various topographies, particularly those that affect the direction of cellular migration. Topographical features, such as ridges and cliffs, were fabricated using multiphoton absorption polymerization. As the cells encountered these topographical features, we tracked their overall motions and shapes, as well as the locations and intensities of certain intracellular signals. We found that when cells undergoing chemokinesis, random migration in response to a chemical signal, encounter a ridge, they tend to move along that ridge, even if the ridge is shorter than the cell. When cells undergoing chemotaxis, directed migration in response to a chemical signal, are directed off of a cliff, they do not fall off the cliff. Instead, they search for new attachment points, eventually change direction, and continue moving along the edge of the cliff. Both ridges and cliffs affect more than just the motion of a cell; they also affect its shape.

11:27AM W39.00002 Cell migration on ridges and cliffs, MEGHAN DRISCOLL, University of Maryland, COLIN MCCANN, University of Maryland and the National Cancer Institute, National Institutes of Health, RAEL KOPACE, JOHN WATTS, University of Maryland, TESS HOMAN, University of Twente, WOLFGANG LOSERT, University of Maryland — The amoeba \(D.\) discoideum is a model system for the study of cellular migration, an important physiological process that occurs in embryonic development, wound healing, and cancer metastasis. We study the motion of \(D.\) discoideum on surfaces with various topographies, particularly those that affect the direction of cellular migration. Topographical features, such as ridges and cliffs, were fabricated using multiphoton absorption polymerization. As the cells encountered these topographical features, we tracked their overall motions and shapes, as well as the locations and intensities of certain intracellular signals. We found that when cells undergoing chemokinesis, random migration in response to a chemical signal, encounter a ridge, they tend to move along that ridge, even if the ridge is shorter than the cell. When cells undergoing chemotaxis, directed migration in response to a chemical signal, are directed off of a cliff, they do not fall off the cliff. Instead, they search for new attachment points, eventually change direction, and continue moving along the edge of the cliff. Both ridges and cliffs affect more than just the motion of a cell; they also affect its shape.

11:39AM W39.00003 ABSTRACT WRITTEN

11:51AM W39.00004 Mutational robustness emerges in a microscopic model of protein evolution¹, KONSTANTIN ZELDOVICH, University of Massachusetts Medical School, EUGENE SHAKHNOCVICH, Harvard University, Department of Chemistry and Chemical Biology — The ability to absorb mutations while retaining structure and function, or mutational robustness, is a remarkable property of natural proteins. We use a computational model of organic evolution [Zeldovich et al, PLOS Comp Biol 3(7):e139 (2007)], which explicitly couples protein physics and population dynamics, to study mutational robustness of evolved model proteins. We compare evolved sequences with the ones designed to fold into the same native structures and having the same thermodynamic stability, and find that evolved sequences are more robust against point mutations, being less likely to be destabilized, and more likely to increase stability upon a point mutation. These results point to sequence evolution as an important method of protein engineering if mutational robustness of the artificially developed proteins is desired. On the biological side, mutational robustness of proteins appears to be a natural consequence of the divergence-mutation- selection evolutionary process.

¹This work is supported by the NIH.

12:03PM W39.00005 Kinetics of Slow Axonal Transport and Shape of Axon¹, PETER JUNG, CHEN YING, YINYUN LI, Department of Physics and Astronomy, Ohio University, ANTHONY BROWN, Center for Molecular Neurobiology and Department of Neuroscience, Ohio State University — The mechanical integrity of the axon in mature axons is provided by neurofilaments(NF). NFs move through the axon at the average slow rate of 0.5mm/day, characterized by bursts of movement and extended pauses in between. The local number of NFs determines the local axonal caliber and as a result, the kinetics of NF movement determines the overall shape of the axon. We developed a kinetic model for movement of NFs based on live cell-imaging (J Neurosci. 2007, 27:507, Mol Biol Cell. 2005, 16:4243). We use this model to predict changes in axonal morphology upon local modifications of the kinetics by e.g. factors released by myelin.

¹This work has been sponsored by NSF under grants IOS-0818412(PJ) and IOS-0818653(AB)

12:15PM W39.00006 Group behavior in cell migration¹, WOLFGANG LOSERT, University of Maryland, CAROLE PARENT, National Cancer Institute, NIH, COLIN MCCANN, University of Maryland and NCI — Cell migration up an external chemical gradient is a crucial element in many biological processes, such as embryogenesis and cancer metastasis. The aim of our study is to quantify chemotaxis of groups of cells. We find that at high cell densities (i.e. low cell-cell distances) cells migrate together in streams either spontaneously or in response to an externally applied chemical gradient. Analysis of cell tracks outside and within streams shows that cells do not speed up or slow down when moving as a group. In addition the persistence of motion appears unaffected by the formation of streams. At large cell-cell distances cells do not form streams in response to externally applied chemical gradients, and fewer cells move. At very low cell plating density cells are unable to respond to a chemical signal, even close to the signal source. We confirm that this lack of motion is not due to signal relay. Our results indicate that a quorum sensing mechanism exists which is closely coupled to chemotaxis.

¹Supported by NSF-PoLS and NCI Intramural Support
1:27PM W39.00010 Effect of Recombination in the Evolutionary Dynamics of HIV under the Surveillance of Immune System. WEIQUN PENG, WENJING YANG, GUANYU WANG, The George Washington University — Human immunodeficiency virus (HIV) is a retrovirus that causes acquired immunodeficiency syndrome (AIDS), which has become one of the most destructive pandemics in history. The fact that HIV evolves very fast plays a central role in AIDS immunopathogenesis and the difficulty we face in finding a cure or a vaccine for AIDS. A distinguishing feature of HIV is its high frequency of recombination. The effect of recombination in the HIV evolution is not clear. We establish a mathematical model of the evolutionary dynamics. This model incorporates both point mutation and recombination for genetic diversity, and employs a fitness function developed by Wang and Deem (PRL 97, 188106, 2006) that accounts for the effect of immune system. Using this model, we explore the role of recombination in the battle between the virus population and the immune system, with a special focus on the condition under which recombination helps the virus population to escape from the immune system.

12:39PM W39.00008 A collective mechanism for phase variation in biofilms1. NICHOLAS CHIA, CARL WOESE, NIGEL GOLDFEN Feld — Understanding how microbes gather into biofilm communities and maintain diversity remains one of the central questions of microbiology, requiring an understanding of microbes as communal rather than individual organisms. Phase variation plays an integral role in the formation of diverse phenotypes within biofilms. We propose a collective mechanism for phase variation based on gene transfer agents, and apply the theory to predict the population structure and growth dynamics of a biofilm. Our results describe quantitatively recent experiments, with the only adjustable parameter being the rate of intercellular horizontal gene transfer. Our approach derives from a more general picture for the emergence of cooperation between microbes.

1This work is partially supported by the Department of Energy through Grant DOE-2005- 05818.

12:51PM W39.00009 ABSTRACT WITHDRAWN —

1:03PM W39.00010 λ-prophage induction modeled as a cooperative failure mode of lytic repression1, NICHOLAS CHIA, University of Illinois at Urbana-Champaign, IDO GOLDING, NIGEL GOLDFEN Feld — We analyze a system-level model for lytic repression of λ-phage in E. coli using reliability theory, showing that the repressor circuit comprises 4 redundant components whose failure mode is prophage induction. Our model reflects the specific biochemical mechanisms involved in regulation, including long-range cooperative binding, and its detailed predictions for prophage induction in E. coli under ultra-violet radiation are in good agreement with experimental data.

1IG - NIH grant R01-GM082837-01A1. NC - DOE grant No. DOE-2005-05818, and the IGB Postdoctoral Fellows Program. IG and NG - NSF Grant No. 082265, PFC: Center for the Physics of Living Cells.

1:15PM W39.00011 Statistical Physics of Vaccine Design, MICHAEL DEEM, Rice University — I will define a new parameter to quantify the antigenic distance between two H3N2 influenza strains. I will use this parameter to measure antigenic distance between circulating H3N2 strains and the closest vaccine component of the influenza vaccine. For the data between 1971 and 2004, the measure of antigenic distance correlates better with efficacy in humans of the H3N2 influenza A annual vaccine than do current state of the art measures of antigenic distance such as phylegetic sequence analysis or ferret antisera inhibition assays. I suggest that this measure of antigenic distance can be used to guide the design of the annual flu vaccine. I will describe combining this measure of antigenic distance with a multiple-strain avian influenza transmission model to study the threat of simultaneous introduction of multiple avian influenza strains. For H3N2 influenza, the model is validated against observed viral fixation rates and epidemic progression rates from the World Health Organization FluNet - Global Influenza Surveillance Network. I find that a multiple-component avian influenza vaccine is helpful to control a simultaneous multiple introduction of bird-flu strains. I introduce Population at Risk (Par) to quantify the risk of a flu pandemic, and calculate by this metric the improvement that a multiple vaccine offers.

1:27PM W39.00012 Spatial coordination in membrane proximal signaling in T-cells. MAXIM N. ARTYOMOV, MIESZKO LIS, ARUP CHAKRABORTY, Massachusetts Institute of Technology — Membrane-proximal signaling initiates signaling networks of the T-cell which ultimately lead to the T-cell activation. Signal formation requires assembly of the several membrane proteins and successful cooperative interactions inside the complex. Diffusion and chemical reactions involved in the process are characterized by substantially different timescales. In this work we consider how the reaction-diffusion system described by the wide spectrum of timescales can be selective for the minute amounts of the signal (cognate peptide-MHC complex) over the large amounts of irrelevant targets (non-cognate peptide-MHC complex). Note that single distinction between relevant and irrelevant targets - the affinity to the T-cell receptor, is nonetheless sufficient to discriminate between two groups of targets. Moreover, proposed mechanism allows for signal cooperativity with non-cognate peptides amplifying the signal from cognate ones even though they can not signal by themselves. This kind of cooperativity has been observed in recent experiments.

1:39PM W39.00013 Digital signaling, signal filters and central tolerance in thymocytes, ASHOK PRASAD, MIT, JULIE ZIKHERMAN, UCSF, JAYAJIT DAS, OSU, JEROEN ROOSE, UCSF, ARTHUR WEISS, UCSF and HHI, ARUP CHAKRABORTY, MIT — T cells are characterized by the antigen binding receptors (TCR’s) they bear. TCR’s carried by immature T cells (thymocytes) are made in the thymus by a stochastic process, followed by testing against self-peptides. Thymocytes that do not respond too strongly die through apoptosis (negative selection). We present a new molecular explanation of this phenomenon via a computational model, which we also tested by experiments. We show that Ras activation in thymocytes is characterized by the presence of a digital molecular switch due to a positive feedback loop in a Ras-activating enzyme. We also show how an important adaptor protein, LAT, acts as a filter, sending weak TCR signals along a pathway that leads to Ras activation via a graded mechanism, and sending stronger signals along another path that activates Ras via the molecular switch. Our model yields a new mechanism for digital signaling of the Erk protein in mammalian cells, and has important implications for autoimmunity.

1:51PM W39.00014 A biophysical model of prokaryotic diversity in geothermal hot springs1. SUZANNE AMADOR KANE, ANNA KLALES, JAMES DUNCAN, ELIZABETH JANUS NETT, Physics Department, Haverford College, Haverford PA 19041 — Photosynthetic bacteria living in geothermal hot spring environments have surprisingly complex ecosystems with an unexpected level of genetic diversity. In particular, their thermal gradients support genetically distinct bacterial strains that differ in their preferred temperatures for reproduction and photosynthesis. Each region along the thermal gradient exhibits multiple strains of photosynthetic bacteria adapted to several distinct thermal optima, rather than the expected single thermal strain adapted to the local environmental temperature. Here we analyze microbiology data from several ecological studies to show that the thermal distribution field data exhibit several universal features independent of location and specific bacterial strain. These include the distribution of optimal temperatures of different thermal strains and the functional dependence of the net population density on temperature. We present a simple population dynamics model of these systems that explains the observed diversity of different strains of the photosynthetic bacteria, the observed thermal population distributions and certain features of population dynamics observed in laboratory studies of the same organisms.

1This work was supported by the Howard Hughes Medical Institute.
2:03PM W30.00015 Understanding Original Antigenic Sin with a Dynamical System. KEYAO PAN, Dept of Bioengineering, Rice Univ, MICHAEL DEEM, Dept of Bioengineering and Physics & Astronomy, Rice Univ — Original antigenic sin is the phenomenon in which prior exposure to an antigen leads to a subsequent suboptimal immune response to a related antigen. Immune memory normally allows for an improved and rapid response to antigens and is the mechanism by which vaccination works. We here develop a dynamical system model of the mechanism of original antigenic sin, clarifying and explaining the detailed spin-glass treatment of original antigenic sin [1]. The dynamical system describes the virus load as it propagates through healthy and infected cells, the naive and memory B cell concentrations, and the affinity of the immune response. Explicit correspondences between the microscopic variables of the spin-glass model and the dynamical system model will be given. The dynamical system model reproduces the phenomenon of original antigenic sin, and describes how competition between different B-cells compromises the overall effect of the immune system. The trade off between the naive and memory immune responses as a function of antigenic distance between the initial and subsequent antigens is displayed. A suboptimal immune response, the original antigenic sin, is observed for intermediate antigenic distances. [1] Deem MW, Lee H-Y. Sequence space localization in the immune system response to vaccination and disease. Phys Rev Lett 2003;91:068101.


11:15AM W40.00000 Crowding Effects on the Unfolding of Ubiquitin1, DAVID PINCUS, Institute For Physical Science and Technology, University of Maryland, DEVARAJAN THIRUMALAI, Director, Biophysics Program, University of Maryland — Using a coarse-grained representation of polypeptide chains, we probed the mechanical stability of Ubiquitin (Ub) monomers and trimers ((Ub)) in the presence of monodisperse spherical crowding agents. Our findings indicate that crowding increases the volume fraction (φc)-dependent average force (⟨f(φc)⟩), relative to the value at φc = 0, needed to unfold Ub and the polypeptide. Furthermore, we found that average unfolding forces increase with decreasing crowder diameter (σc). The average unfolding force (f(φc)) depends on the ratio σc/σ, where D ∝ σc(σc/σ)2 with R Each being the radius of gyration of Ub (or (Ub)) in the unfolded state. Examination of the unfolding pathways shows that, relative to φc = 0, crowding promotes reassociation of ruptured secondary structural elements. Both the nature of the unfolding pathways (f(φc)) for (Ub) are altered in the presence of crowding particles with the effect being most dramatic for the subunit that unfolds last. We predict that (f(φc)) scales in a simple manner with φc.

1Supported by National Science Foundation (grant EPS-0314742) and the West Virginia University WVNano Initiative.

11:27AM W40.00002 Electron Transfer in Myoglobin-based Single-Electron Transistors1, DEBIN LI, Dept. of Physics, West Virginia University, PETER GANNETT, Basic Pharmaceutical Sciences, West Virginia University, DAVID LEDERMAN, Dept. of Physics, West Virginia University — The mechanism of electron transfer by myoglobin was investigated using nanometer-gap platinum electrodes fabricated by breaking a small junction by electromigration at cryogenic temperatures. The experimental results suggest single electron transport behavior is mediated by resonance of the electronic levels of the heme group in a single myoglobin protein. Evidence for a two-step electron tunneling process, resulting from the structural relaxation of the protein with the addition of a single electron, was observed. Our experimental results show that the slow protein relaxation may result in resonant tunneling and the fast protein relaxation is the condition of two-step resonant tunneling behavior. The conformation and orientation of myoglobin in the gap of electrodes may significantly affect the conductance of these devices. The calculation for the conductance graph as a function of gate voltage and bias voltage was performed with the rate equations for electron tunneling via discrete quantum states and considering the two-step process. The results of calculation match those of our experiment.

11:39AM W40.00003 Surface-enhanced photocycle studied in a single photoreceptor protein molecule, KAAN KALKAN, AIHUA XIE, Oklahoma State University — Photoactive yellow protein (PYP) functions as a blue light sensor for bacterial vision (phototaxis). The photocycle of PYP is initiated by the absorption of a blue photon (absorption peak at 446 nm) by its para-coumaric acid (pCA) chromophore. The photon energy is stored in the pCA through photoisomerization which is subsequently transferred to the rest of the protein through a series of conformational states, finally leading to its partial unfolding (signaling). The present work captures the distinct conformational changes of PYP at the single molecule level, during the execution of its photocycle. In particular, the present work employs surface-enhanced Raman scattering (SERS) active substrates and non-resonant excitation at 514 nm. As we confirm with regular Raman spectroscopy, the photocycle of PYP cannot be excited under 514 nm irradiation. On the contrary, 514 nm photons can excite the photocycle when PYP is adsorbed on silver, as we evidence from single molecule as well as ensemble-averaged SERS. In this case, the optical absorption of PYP shows a dramatic broadening (full width at half maximum shifting from 0.4 to 0.9 eV) such that electronic excitation can occur significantly at 514 nm. Therefore, the origin of the observed “surface-enhanced photocycle” is understood to be of the same as “chemical enhancement” in SERS in view of the “adsorbate-induced resonance states model” (Persson, 1993).

11:51AM W40.00004 Rigidity effects and mechanical unfolding of proteins, OLEG VOROV, DENNIS LIVESAY, DONALD JACOBS, University of North Carolina, Charlotte — We describe a new method that shows promise for evaluating the partition function for a protein under an applied external force within a Distance Constraint Model (DCM). This approach is based on an approximate account for the rigidity effects due to hydrogen bond crosslinking using Maxwell constraint counting. Within a mean-field treatment, the free energy is estimated accurately over an ensemble of accessible conformations conditional upon the breaking of various weakest-link distance constraints, as they successively break due to a series of minu structural transitions. These calculations are performed using an exact transfer matrix approach combined with a combinatorial partitioning of the structure into different parts based on separating lines of unfolding pathways. The various shortest paths over an ensemble of structures that “crack” open in different ways are used to obtain the appropriate Boltzmann weight, related to the work done by the external pulling force. For structures with beta-hairpin geometry, all permutations of unfolding pathways are enumerated exactly. For a simple minimal DCM, results for extension-force curves agree markedly well with experiment.

12:03PM W40.00005 Physical Principles of Virus Templating through Single Molecule Dynamic Force Spectroscopy, RAYMOND FRIDDE, SELIM ELHADJ, GEORGE GILMER, ALEKSANDR NOY, LLLNL, JAMES DE YOREO, Molecular Foundry, LBNL — The use of macromolecular scaffolds for hierarchical organization of molecules and materials is a common strategy in living systems that leads to emergent behavior. One characteristic of this strategy is that it generates micron-scale structures from nm-scale building blocks, possessing high-density functionality, defined at angstrom-scales by active sites; a typical example being viral capsids. We are systematically determining the physical variables necessary to consistently pattern virus particles on to nanoscale templates. This presentation will focus on our theoretical and experimental findings regarding our Dynamic force spectroscopy (DFS) measurements; a technique in which fundamental parameters related to interaction potentials can be determined. Here we present a novel theory for determining kinetic desorption rates and equilibrium free energies using DFS in which two well-defined states exist. We compare the results with force spectra measured between individual MS2 virions and chemically modified AFM tips. We also investigate the effects of solution additives, such as PEG, on microscopic kinetics and free energies. Finally, we discuss the relation of single-molecule measurements with the ensemble, and show a connection between the two in the case of biomolecular dissociation.
12:15PM W40.00006 Probing Protein Folding Kinetics with High-resolution, Stabilized Optical Tweezers. WESLEY WONG, KEN HALVORSEN, Harvard University — Single-molecule techniques provide a powerful means of exploring molecular transitions such as the unfolding and refolding of a protein. However, the quantification of bi-directional transitions and near-equilibrium phenomena poses unique challenges, and is often limited by the detection resolution and long-term stability of the instrument. We have developed unique optical tweezers methods that address these problems, including an interference-based method for high-resolution 3D bead tracking (≈ 1 nm laterally, ≈ 0.3 nm vertically, at > 100 Hz), and a continuous autofocus system that stabilizes the trap height to within 1-2 nm long-term [1,2]. We have used our instruments to quantify the force-dependent unfolding and refolding kinetics of single protein domains (e.g. spectrin in collaboration with E. Evans). These single-molecule studies are presented, together with the accompanying probabilistic analysis that we have developed. References: 1. W.P. Wong, V. Heinrich, E. Evans, Mat. Res. Soc. Symp. Proc., 790, P5.1-P5.10 (2004). 2. V. Heinrich, W.P. Wong, K. Halvorsen, E. Evans, Langmuir, 24, 1194-1203 (2008).

12:27PM W40.00007 Electrostatic signatures of single protein dynamics for detection with carbon nanotube sensors. G. SCHNEIDER, L. PRISBREY, E. MINOT, Oregon State University — Observing single molecule dynamics in real time at atomic resolution is crucial to study enzyme function, which is closely linked to the intrinsic dynamics of the enzyme and molecular interactions between enzyme and substrate. At present, techniques such as nuclear magnetic resonance (NMR) and single molecule fluorescence energy transfer (FRET) are used together with computer simulations to study single molecule dynamics. Recent progress in point-functionalization of single wall carbon nanotube (CNT) opens the possibility of electronic detection of single molecule dynamics [2]. CNTs are ideal candidates for electronic sensing of single protein dynamics. Typical CNT diameters are 1-2 nm, comparable to both the size of proteins in solution and the electrostatic screening length in physiological solutions. CNT sensors based on point defects have potential advantages over FRET including better time resolution. We report results for the electrostatic signature of several proteins in solution, both in substrate free and bound forms, and discuss the potential for electronic detection of biologically relevant single protein dynamics using functionalized carbon nanotubes.

12:39PM W40.00008 Experimental Investigation of the Velocity Convergence of Jarzynski’s Equality Using Single-Molecule AFM Pulling of Titin I27. NOLAN HARRIS, CHING-HWA KIANG, Rice University, Physics and Astronomy Department, Houston, TX 77005 — Single molecule atomic force microscopy (AFM) of individual biomolecules allows one to observe high energy conformations and transitions between equilibrium states that are not otherwise observable. Jarzynski’s equality has been used to extract important equilibrium information, such as free energy surfaces, from these nonequilibrium AFM measurements. However, the convergence behavior of Jarzynski’s equality, i.e. the number of AFM trajectories required to adequately sample the nonequilibrium work distribution of a process, depends nontrivially on the AFM pulling schedule. Here we study the velocity dependent nature of Jarzynski’s equality in AFM experiments. We reconstructed the free energy surfaces for the forced unfolding of the I27 domain of human cardiac titin via AFM using different pulling velocities. We found that the number of experimental trajectories required for convergence of Jarzynski’s equality increases roughly exponentially as experimental pulling velocity is increased. We suggest optimal pulling velocities for pulling titin I27 and discuss the obstacles involved with using extreme pulling velocities.

12:51PM W40.00009 Real Time Single Molecule Imaging of Protein-Surface Interactions. SHANNON KIAN G. ZAREH, SHAWN H. DECENTZO, Y.M. WANG, Washington University in St.Louis, USA 63130 — We study the dynamics of the adsorption of protein to surfaces using real time Total Internal Reflection Fluorescence microscopy (TIRF). We have observed two mechanisms responsible for protein adsorption on surfaces: Reversible and Irreversible binding. The reversible binding occurs on the deposition step induced by the initial deposition flow, and the reversible binding is the equilibrium binding between the proteins and the surfaces. Our study has shown that the irreversible binding is the main contribution to the surface adsorption of proteins. We will discuss the energy for GFP and fused-silica surface interaction, and also a method to prevent protein adsorption onto surfaces.

1:03PM W40.00010 Single molecule image deconvolution. I. Standard deviation analysis of immobile fluorescent molecules. MICHAEL C. DESANTIS, SHAWN H. DECENTZO, Y.M. WANG, Washington University, St. Louis, MO — Single molecule fluorescence imaging has been a powerful technique in studying individual processes not accessible by bulk, ensemble-averaged measurements [1]. Improvements in image analysis are required for high temporal and spatial precision in the localization of single fluorescent molecules. We present the first thorough standard deviation analysis for point spread functions (PSFs) of single immobile fluorescent molecules. Using this new single molecule image deconvolution (SMID) method, we show that 3D localization of individual molecules with sub-nanometer precision can be achieved. We have derived an expression estimating the standard error of the PSF’s standard deviation, incorporating experimental effects of the number of collected photons, finite pixel size, and background noise. The localization precision obtained via this expression is approximately 1.5 times better than the current available methods. The use of SMID to extract subexposure dynamics of mobile molecules will also be discussed.

1:15PM W40.00011 Monte Carlo simulation of single-molecule trapping via electrophoresis. WILLIAM ROBINSON, LLOYD DAVIS, UTSI — For many biophysical studies, there is a need to observe a molecule for an extended duration without immobilizing it on a surface. The problem of trapping a single fluorescent molecule in solution is examined here via Monte Carlo numerical simulation. Optical forces are insufficient for trapping small molecules. Instead, trapping is executed by sensing the position and applying real-time feedback of flow to compensate diffusional displacement. Using a nanochannel as the volume of interest reduces the problem to one dimension, and with such a configuration the position of the molecule can be measured from its fluorescence in the presence of a two-focus irradiance pattern. The collected photons are analyzed by an algorithm developed previously. Two stable trajectories are obtained, indicating that the molecule is immobilized on a surface without photobleaching. Preliminary results and further applications will be presented.

1:27PM W40.00012 Sub-diffraction limit differentiation of single fluorophores using Single Molecule Image Deconvolution (SMID). SHAWN H. DECENTZO, MICHAEL C. DESANTIS, Y. M. WANG, Department of Physics Washington University, St. Louis Missouri, 63130 USA — In order to better understand biological systems, researchers demand new techniques and improvements in single molecule differentiation. We present a unique approach utilizing an analysis of the standard deviation of the Gaussian point spread function of single immobile fluorescent molecules. This technique, Single Molecule Image Deconvolution (SMID), is applicable to standard TIRF instrumentation and standard fluorophores. We demonstrate the method by measuring the separation of two Cy3 molecules attached to the ends of short double-stranded DNA immobilized on a surface without photobleaching. Preliminary results and further applications will be presented.
1:39PM W40.00013 Selection of optimal variants of Go-like models of proteins through studies of stretching, JOANNA SULKOWSKA, Center of Theoretical Biological Physics, Department of Physics, UCSD, and Institute of Physics Polish Academy of Science, Poland, MAREK CIEPLAK, Institute of Physics Polish Academy of Science, Al. Lotnikow 32/48, Warsaw, Poland — The Go-like models of proteins are constructed based on the knowledge of the native conformation. However, there are many possible choices of a Hamiltonian for which the ground state coincides with the native state. Here, we propose to use experimental data on protein stretching to determine what choices are most adequate physically. This criterion is motivated by the fact that stretching processes usually start with the native structure, in the vicinity of which the Go-like models should work the best. Our selection procedure is applied to 62 different versions of the Go model and is based on 28 proteins. We consider different potentials, contact maps, local stiffness energies, and energy scales — uniform and non-uniform. In the latter case, the strength of the nonuniformity was governed either by specificity or by properties related to positioning of the side groups. Among them there is the simplest variant: uniform couplings and no i + 2 contacts. This choice also leads to good folding properties in most cases. We elucidate relationship between the local stiffness described by a potential which involves local chirality and the one which involves dihedral and bond angles. The latter stiffness improves folding but there is little difference between them when it comes to stretching.

1:51PM W40.00014 Discontinuities at the DNA supercoiling transition, BRYAN DANIELS, SCOTT FORTH, MAXIM SHEININ, MICHELLE WANG, JAMES SETHNA, LASSP, Cornell University — While slowly turning the ends of a single molecule of DNA at constant applied force, a discontinuity was recently observed at the supercoiling transition, when a small plectoneme is suddenly formed. This can be understood as an abrupt transition into a phase in which stretched and plectonemic DNA coexist. We argue that there should be discontinuities in both the extension and the torque at the transition, and provide experimental evidence for both. To predict the sizes of these discontinuities and how they change with the overall length of DNA, we organize a theory for the coexisting plectonemic state in terms of four length-independent parameters. We also test plectoneme theories, including our own elastic rod simulation, finding discrepancies with experiment that can be understood in terms of the four coexisting state parameters.

2:03PM W40.00015 Pressure-driven single-file transport of DNA molecules along linear arrays of nanopits embedded in a slit-like nanochannel,1, JACKSON DEL BONIS-O’DONNELL, WALTER REISNER, Brown University, ANDERS KRISTENSEN, Technical University of Denmark, DEREK STEIN, Brown University — Due to the growth in nanobiofluidic technology for DNA manipulation and analysis, there is a growing interest in understanding the physics of DNA in nanoconfined environments. Using fluorescence video microscopy we study the transport of DNA in slit-like nanochannels with an embedded nanotopology consisting of linear arrays of nanopit structures. The nanopit structures are made via a two level fabrication process: (1) An e-beam lithography and etching step to make the nanopits followed by (2) a photolithography step to fabricate the slit. Under an applied pressure drop the DNA molecules are observed to move single-file down the nanopit array undergoing sequential pit-to-pit hops. We make systematic measurements of pressure dependent nanopit velocity. We observe two distinct transport regimes depending on whether the molecule configuration can occupy a single pit or must subdivide multiple pits. We interpret our results in terms of a simple scaling picture of the free energy of chains in the linear array.

1 NSF Grant #0805176

Thursday, March 19, 2009 11:15AM - 1:51PM — Session W41 DCMP: Kondo Physics; Dynamical Mean-Field Theory 413

11:15AM W41.00001 The 2d Kondo effect in p-type Quantum Wells in GaAs, THEODORE CASTNER, University of Rochester — Two groups [Huang et al. [1] and Hamilton et al. [2]] have observed minima in the resistivity \( \rho(T) \) at very low T well below \( \rho_{\text{max}} \) at \( T_{\text{max}} \) in metallic samples (\( p > p_c \)). Minima in [1] were found at 32 mK for \( p \sim 2.1 \) mK, 25 mK for \( p \sim 1.76 \) mK, while no minimum was observed down to 0.5 mK for \( p \sim 1.24 \) mK. Both groups have interpreted their results in terms of a crossover to insulating (nonmetallic) behavior for \( T < T_{m} \) where \( dp/dT < 0 \). An alternative explanation arises from a 2d Kondo effect. Using the Hamann function [3] for the magnetic scattering contribution from localized magnetic moments and a term \( m(1/CT)F(p) \) from screening interactions one obtains an expression for \( T_{\text{m}}(p) \) which is very close to the Kondo temperature \( T_{K}(p) \) given by \( (E_{F}/k)\exp(-1/N(E_F)) \). The very strong p-dependence of \( T_{\text{m}}(p) \) and \( T_{K}(p) \) is dominated by \( N(E_F) \) which is shown to approach zero as \( p \) approaches \( p_c \) because of the pseudogap in the DOS. Good agreement is obtained \( T_{\text{m}}(p) \) for both [1] and [2]. The data in [1] supports metallic behavior down to 0.5 mK. The implications for a 2d MIT as a QPT are discussed.

11:27AM W41.00002 Quantum phase transition in the XY-anisotropic Bose-Fermi Kondo model, MENGXING CHENG, KEVIN INGERSENT, University of Florida — Using the numerical renormalization group, we study the quantum phase transition induced by dissipation in the XY-anisotropic Bose-Fermi Kondo model for a spin-one-half magnetic impurity coupled both to the on-site spin of a conduction electron band and, via its x and y spin components, to a bath of vector bosons. We focus on the case of a sub-Ohmic bath characterized by a power-law spectral exponent \( s < 1 \). Upon increasing the coupling of the impurity to the bosonic bath (at fixed fermionic coupling), the system exhibits a continuous quantum phase transition from a Kondo-screened ground state to a state in which the impurity moment is localized by the dissipation. We probe the quantum-critical behavior in the vicinity of this transition through the calculation of critical exponents describing the static and dynamical response to a local magnetic field both at absolute zero and at finite temperatures. Critical comparisons are made with analytical renormalization-group results obtained previously through expansion around the Ohmic case \( s = 1 \).

1 Supported by NSF Grant DMR-0701050

11:39AM W41.00003 ABSTRACT WITHDRAWN

11:51AM W41.00004 Validity of Equation-of-Motion Approach to Kondo Problem in the Large N limit, YUNONG QI, Texas Center for Superconductivity, University of Houston, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory, CHIN-SEN TING, Texas Center for Superconductivity, University of Houston — The Anderson impurity model for Kondo problem is investigated for arbitrary orbit-spin degeneracy \( N \) of the magnetic impurity by the equation of motion method (EOM). By employing a new decoupling scheme, a set self-consistent equations for the one-particle Green function are derived and numerically solved in the large-\( N \) approximation. For the particle-hole symmetric Anderson model with finite Coulomb interaction \( U \), we show that the Kondo resonance at the impurity site exists for all \( N \geq 2 \). The approach removes the pathology in the standard EOM for \( N = 2 \), and has the same level of applicability as non-crossing approximation. For \( N = 2 \), an exchange field splits the Kondo resonance into only two peaks, consistent with the result from more rigorous numerical renormalization group (NRG) method. The temperature dependence of the Kondo resonance peak is also discussed.

1 We here should give special thanks to Shufeng Zhang and R. C Albers for useful discussions. This work was supported by the Robert Welch Foundation No. E-1146 at the University of Houston (Y.Q. and C.S.T.), by U.S. DOE under Contract No. DE-AC52-06NA25396.
12:03PM W41.00005 Evolution of a Large Fermi Surface in the Kondo Lattice  . JUNYA OTSUKI, Tohoku University, HIROAKI KUSUNOSE, Ehime University, YOSHIO KURAMOTO, Tohoku University — We investigate the Kondo lattice model with use of the continuous-time quantum Monte Carlo method, combined with the dynamical mean-field theory. The antiferromagnetic phase diagram is determined from a divergency of the corresponding susceptibility [1]. In the paramagnetic phase, crossover behavior is traced quantitatively to a heavy Fermi-liquid state from the local-moment state at high temperatures [2]. The momentum distribution in the low-temperature limit acquires a discontinuity at the location that involves the local-spin degrees of freedom. Even without the charge degrees of freedom for local electrons, the excitation spectra exhibit hybridized bands similar to those in the Anderson lattice. Temperature dependence in the zero-energy component of the self-energy is crucial in forming the Fermi-liquid state with the large Fermi surface. [1] J. Otsuki, H. Kusunose and Y. Kuramoto, arXiv:0808.3829; arXiv:0811.1102. [2] J. Otsuki, H. Kusunose and Y. Kuramoto, arXiv:0811.2613 to appear in Phys. Rev. Lett.

12:15PM W41.00006 A linear in $\beta$ solver for Cluster Dynamical Mean Field Theory . EHSAN KHATAMI, MARK JARRELL, University of Cincinnati, CHE-RUNG LEE, National Tsing Hua University, RICHARD SCALETTRAR, University of California, Davis — We develop a Quantum Monte Carlo (QMC) cluster solver for the Dynamical Cluster Approximation (DCA) which scales linearly in the inverse temperature, $\beta$, and has the same minus sign problem as conventional methods. Determinantal QMC (DQMC) used in this method is modified by adding non-interacting bands to mimic the coupling to the host. The DCA hybridization function is fitted to the non-interacting band parameters. We prove that the sign problem has the same statistics as in the Hirsch-Fye (HF) algorithm in the limit of a large number of bath bands ($N_b$). Whereas the HFQMC scales as $\beta^3$, this DQMC-based method scales linearly in $\beta$. We demonstrate rapid convergence of the sign to the HF result for different cluster sizes and model parameters as $N_b$ increases. We also present results for the convergence of other physical quantities to their HFQMC counterparts. This method can be used to solve other embedded cluster problems including those in Dynamical Mean Field Theory (DMFT), and cellular DMFT.

12:27PM W41.00007 The relationship between Hirsch-Fye and weak coupling diagrammatic Quantum Monte Carlo methods . KARLIS MIKELSONS, ALEXANDRU MACRIDIN, University Of Cincinnati, MARK JARRELL, Rutgers University — Two weak coupling Continuous Time Quantum Monte Carlo (CTQMC) methods are shown to be equivalent for Hubbard-like interactions. A relation between these CTQMC methods and the Hirsch-Fye Quantum Monte Carlo (HFQMC) method is established, identifying the latter as an approximation within CTQMC and providing a diagrammatic interpretation of HFQMC. Both HFQMC and CTQMC are shown to be equivalent when the number of time slices in HFQMC becomes infinite, implying the same degree of fermion sign problem in this limit.

12:39PM W41.00008 Cluster Dynamical Mean Field Theory of the Mott Transition . HYOWON PARK, KRISTJAN HAULE, GABRIEL KOTLIAR, Rutgers University — We address the nature of the Mott transition in the Hubbard model at half-filling using cluster dynamical mean field theory (DMFT). We compare cluster DMFT results with those of single site DMFT. We show that inclusion of the short range correlations on top of the on-site correlations does not change the order of the transition between the paramagnetic metal and the paramagnetic Mott insulator, which remains first order. However, the short range correlations reduce substantially the critical $U$ and modify the shape of the transition line. Moreover, they lead to very different physical properties of the metallic and insulating phases near the transition point. Approaching the transition from the metallic side, we find an anomalous metallic state with very low coherence scale. The insulating state is characterized by the narrow Mott gap with pronounced peaks at the gap edge.

12:51PM W41.00009 Nearly frozen Coulomb liquids . YOHANES PRAMUDYA, SERGEY PANKOV, Florida State University, National High Magnetic Field Laboratory, EFFRATIOS MANOUSAKIS, Florida State University, MARTECH, VLADIMIR DOBROSavljevic, Florida State University, National High Magnetic Field Laboratory — We show that very long range repulsive interactions of a generalized Coulomb-like form $V(R) \sim R^{-\alpha}$, with $\alpha < d$ (d-spatial dimensionality), typically introduce very strong frustration, resulting in extreme fragility of any charge-ordered state. An “almost frozen” liquid then survives in a broad dynamical range above the (very low) melting temperature $T_c$. Using a combination of extended dynamical mean-field theory [1] and Monte Carlo simulations we study classical lattice gas models with such long range interaction, focusing on the behavior at $T > T_c$. We find that a soft, temperature-dependent pseudo-gap emerges in this regime, reflecting strong short-range correlations that persist above the melting temperature. This “pseudo-gap” phase is characterized by unusual insulating-like, but very weakly temperature dependent transport, similar to experimental findings [2] in many low carrier density systems. [1] S.Pankov and V. Dobrosavljevic, Phys. Rev. Lett. 94, 046402 (2005). [2] K. Lai, W. Pan, D. C. Tsui, S. Lyon, M. Muhlbberger, and F. Schaffler, Phys. Rev. B 75, 033314 (2007).

1:03PM W41.00010 Quantum criticality out of equilibrium: Thermopower and shot noise in a ferromagnetic single electron transistor . JEDEDIAH PIXLEY, STEFAN KIRCHNER, QIMIAO SI, Rice University — The low-energy properties of a single electron transistor attached to ferromagnetic leads are described by the Bose-Fermi Anderson model. This model can undergo a continuous phase transition and it was shown in [1] that the transistor can be tuned through this quantum phase transition. The out-of-equilibrium scaling properties near the quantum critical point and in the adjacent phases of the spin and charge response and their fluctuation-dissipation ratios were recently studied in [2]. In this contribution, we study the thermopower and shot noise, which probe the quantum criticality in a way that goes beyond the current-voltage characteristics. The thermoelectric properties of a quantum dot in the Kondo regime can be directly measured [3]. Bulk thermopower measurements of heavy fermion compounds near their quantum critical point and in the adjacent phases of the spin and charge response and their fluctuation-dissipation ratios were recently presented (2005). We find an anomalous metallic state with very low coherence scale. The insulating state is characterized by the narrow Mott gap with pronounced peaks at the gap edge.

1:15PM W41.00011 Mottness scenario for non-Fermi liquid behavior in the periodic Anderson model within dynamical mean-field theory . GIOVANNI SORDI, ADRIANO AMARICCI, MARCELO ROZENBERG, Laboratoire de Physique des Solides, CNRS-UMR8502, Université de Paris-Sud, Orsay 91405, France — We study the Mott metal-insulator transition in the periodic Anderson model within dynamical mean-field theory (DMFT). Near the quantum transition, we find a non-Fermi liquid metallic state down to a vanishing temperature scale. We identify the origin of the non-Fermi liquid behavior as due to magnetic scattering of the doped carriers by the localized moments. The non-Fermi liquid state can be tuned by either doping or external magnetic field. Our results show that the coupling to spatial magnetic fluctuations (absent in DMFT) is not a prerequisite to realize a non-Fermi liquid scenario for heavy fermion systems. Refs: Phys. Rev. Lett. 99, 196403 (2007); Phys. Rev. Lett. 101, 146403 (2008).
1:27PM W41.00012 Percolation transition in nanowire magnetorheological fluids1. JOSH KARLI, DARIN ZIMMERMAN, JOSEPH FILER, RICHARD BELL. The Pennsylvania State University, Altoona, NORMAN WERELEY, The University of Maryland — We measure the yield stress of magnetorheological (MR) fluids that employ cobalt nanowires as the ferromagnetic component and observe a percolation transition in the yield stress at a critical value of the cobalt-nanowire volume fraction, \( p_c \). The critical volume fraction depends not only on the particle size and aspect ratio (as expected) but also on the external magnetic field applied to the MR-fluid sample. We fit the yield-stress data using McLachlan’s generalized effective medium (GEM) model to determine \( p_c \) and the percolation exponents \( x \) and \( t \) that describe the transition behavior below and above \( p_c \), respectively. The phase transition from low- to high-yield stress at low magnetic-particle volume fraction (< 1%) has potential application to the development of precision magnetic sensors and actuators.

1This work was supported by grants from the National Science Foundation (NSF-RUI: CBET-0755696) and Altoona College.

1:39PM W41.00013 Anderson localization transition in thin films of gadolinium1. R. MISRA, A.F. HEBARD, K.A. MUTTALIB, University of Florida, Gainesville, FL-32611, USA, P. WOELFLE, ITKMI, University of Karlsruhe, Germany — In situ temperature-dependent transport studies have been performed on a series of gadolinium (Gd) films deposited onto sapphire substrates having sheet resistance \( R_0 \equiv R_{xx}(5K) \) varying over the range 4011 \( \Omega \) (∼35Å) to 132 KΩ (∼20 Å). The disorder strength, as measured by \( R_0 \), is sufficiently high so that quantum corrections to the classical Boltzmann conductivity are no longer observed. In this region of moderately strong disorder, we find a temperature-dependent conductivity of the form \( \sigma(T) = A + BT^p \) where \( A \) and \( B \) are disorder-dependent constants and \( p \) is a power with value 0.4. We find that \( A \) is proportional to \((1-R_0/R_c)^{-t} \) where the conductivity exponent \( s = -1 \) and the critical resistance \( R_c = 22.7 \Omega \). This change in sign of \( A \) with unity exponent at critical disorder describes the critical regime of an Anderson localization transition[1] with the temperature-dependent localization length sufficiently small so that the Gd films can be considered to be in the 3D regime, rather than the 2D regime where metallic behavior does not occur [2]. [1] Lee & Ramakrishnan, RMP 57, 287 (1985); Belitz & Kirkpatrick, RMP 66, 261 (1994) [2] Abrahams, Anderson, Licciardello & Ramakrishnan, PRL 42, 673 (1979)
4:18PM X1.00004 Effect of pair-breaking on superconductivity and on persistent currents well above the transition temperature, L. Bulaevskii (LANL), U. Welp, C. Kurter, K. Gray (MSD, ANL), L. Ozyuzer (Izmir Institute of Technology, Turkey), K. Kadowaki

We study the low temperature phase diagram of the vortex matter in the high-T_c superconductor Bi_2Sr_2CaCu_2O_8+δ. By employing vortex shaking the vortex system is relaxed towards the equilibrium state. We thus reveal a novel second-order glass transition, manifested by a sharp reversible kink in the measured local magnetization. The glass line bisects the first-order melting line close to its extremum below which disorder is dominant. Consequently, the phase diagram consists of four thermodynamic phases: At high fields, above the melting line, we find amorphous vortex glass and liquid phases; Surprisingly, at low fields the glass transition separates between a low-temperature Bragg glass and a thermally depinned variant of it - possibly a perfect lattice. Studying the oxygen doping dependence of the vortex phase diagram we unexpectedly find that the novel low-temperature glass transition, along which quenched disorder should play a dominant role, has the same anisotropy dependence as that of the high-temperature melting line, where disorder is negligible. Finally, we utilize an indirect measurement technique to reconstruct the low-temperature I-V characteristics in the region which is inaccessible by transport measurements. At high temperatures the bulk resistance is of a thermally activated flux flow with linear I-V both in the liquid phase above the melting line as well as below it within the ordered phase. At lower temperatures, on approaching the glass transition, the temperature dependence of the bulk resistance becomes much sharper. This deviation from a simple Arrhenius behavior tracks the glass line, and may signify criticality.

1H. Beidenkopf is supported by the Adams Fellowship Program of the Israel Academy of Sciences and Humanities

4:54PM X1.00005 Paramagnetic or diamagnetic persistent currents? A topological point of view, Xavier Waintal, SPEC, CEA Saclay — A persistent current flows at low temperatures in small conducting rings when they are threaded by a magnetic flux. I will discuss the sign of this persistent current (diamagnetic or paramagnetic response) in the special case of N electrons in a one dimensional ring. One dimension is very special in the sense that the sign of the persistent current is entirely controlled by the topology of the system. I will establish lower bounds for the free energy in the presence of arbitrary electron-electron interactions and external potentials. Those bounds are the counterparts of upper bounds derived by Leggett using another topological argument. Rings with odd (even) numbers of polarized electrons are always diamagnetic (paramagnetic).

The situation is more interesting with unpolarized electrons where Leggett upper bound breaks down: rings with N = 4n exhibit either paramagnetic behavior or a superconductor-like current-phase relation. The topological argument provides a rigorous justification for the phenomenological Huckle rule which states that cyclic molecules with 4n ± 2 electrons like benzene are aromatic while those with 4n electrons are not.


Thursday, March 19, 2009 2:30PM - 4:54PM –
Session X2 DCMP: Vortex Dynamics and Josephson Lasers in Superconductors Spirit of Pittsburgh Ballroom BC

2:30PM X2.00001 Thermodynamics and Flow of the Vortex Matter at the Second-Order Glass Transition in Bi_2Sr_2CaCu_2O_8+x, HAIM BEIDENKOPF, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — We study the low temperature phase diagram of the vortex matter in the high-T_c superconductor Bi_2Sr_2CaCu_2O_8. By employing vortex shaking the vortex system is relaxed towards the equilibrium state. We thus reveal a novel second-order glass transition, manifested by a sharp reversible kink in the measured local magnetization. The glass line bisects the first-order melting line close to its extremum below which disorder is dominant. Consequently, the phase diagram consists of four thermodynamic phases: At high fields, above the melting line, we find amorphous vortex glass and liquid phases; Surprisingly, at low fields the glass transition separates between a low-temperature Bragg glass and a thermally depinned variant of it - possibly a perfect lattice. Studying the oxygen doping dependence of the vortex phase diagram we unexpectedly find that the novel low-temperature glass transition, along which quenched disorder should play a dominant role, has the same anisotropy dependence as that of the high-temperature melting line, where disorder is negligible. Finally, we utilize an indirect measurement technique to reconstruct the low-temperature I-V characteristics in the region which is inaccessible by transport measurements. At high temperatures the bulk resistance is of a thermally activated flux flow with linear I-V both in the liquid phase above the melting line as well as below it within the ordered phase. At lower temperatures, on approaching the glass transition, the temperature dependence of the bulk resistance becomes much sharper. This deviation from a simple Arrhenius behavior tracks the glass line, and may signify criticality.

3:06PM X2.00002 Nanomechanics of Individual, Isolated Vortices in a Cuprate Superconductor, KATHRYN MOLER, Stanford University — No abstract available.

3:42PM X2.00003 Structure and stability of dynamic coherent states in intrinsic Josephson-junction stacks, ALEXEI KOSHELEV*, Materials Science Division, Argonne National Laboratory — Intrinsic Josephson-junction stacks are realized in mesas fabricated out of high-temperature superconductors. Phase oscillations in different junctions can be synchronized via coupling to the intrinsic cavity mode leading to powerful electromagnetic radiation in terahertz frequency range. As homogeneous oscillations do not couple directly to the cavity modes, the mechanism of mode excitations is a nontrivial issue. New inhomogeneous dynamic state providing such coupling has been demonstrated recently. In this state, the stack spontaneously splits into two subsystems with different phase-oscillation patterns. The phase shift between the oscillations in the two subsystems depends on the order parameter and on the external fields. The formation of this state can be used for efficient pumping of the energy into the cavity resonance. We will also discuss (i) stability of coherent states (ii) synchronization in inhomogeneous mesas, and (iii) mechanisms of damping of the resonance mode.

[4] In collaboration with L. Bulaevskii (LANL), U. Welp, C. Kurter, K. Gray (MSD, ANL), L. Ozyuzer (Izmir Institute of Technology, Turkey), K. Kadawaki (Tsukuba University, Japan)

This work was supported by the U. S. DOE, Office of Science, under contract # DE-AC02-06CH11357.
Radiation is the frequency, \( f \), of the radiation depends strongly on the shape and the size of the mesa. In the case of rectangular shape it follows the relation, \( f = c/(2\pi n) \), where \( c \) is the velocity of light in vacuum, \( n \) the refractivity of the superconductor and \( w \) the width of the mesa (shorter edge dimension), while it only depends on the radius \( a \) in the case of cylindrical mesa. Higher harmonics are also observed. Another stringent requirement for the radiation is the uc-Josephson effect, which must be fulfilled in each junction with the same frequency determined by the equation: \( fh = 2eV/n = 2e\nu_o \), where \( V \) is the voltage across the whole junction, \( N \) the number of junctions involved in the mesa, \( \nu_o \) the voltage appearing between each junctions, \( h \) the Planck constant, \( e \) the elementary charge. Since the radiation is monochromatic, \( \nu_o \) must be identical and synchronized coherently in all junctions in the mesa. A simple phenomenological interpretation of this synchronization is that it may occur due to the cavity resonance effect inside the mesa. The peculiar temperature dependence and the anisotropic directivity of radiation power observed experimentally may give a hint to understand the mechanism of such synchronized THz radiation from intrinsic Josephson junctions. We think that nonlinearity to be inherent in the Josephson junction as well as thermal nonequilibrium effect plays a crucial role for the synchronized THz oscillation. A more detailed view for the mechanism based on the experimental results will be presented.

1. This work has been supported by KAKENHI, Grant-in-Aid for Scientific Research (A) (18204031), the Ministry of Education, Culture, Sports, Science and Technology (MEXT), JAPAN, CREST JST, WPI at NIMS (MANA), and JSPS Core-to-Core Program.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X3 DCMP: Spin Hall and Quantum Spin Hall Effects 301/302

2:30PM X3.00001 Imaging electrical spin generation and spin Hall dynamics in semiconductors1, N.P. STERN2, Center for Spintronics and Quantum Computation, University of California, Santa Barbara, CA 93106 — The capability to generate and manipulate spin polarization through the spin-orbit interaction drives interest in all-electrical techniques to exploit electron spins for semiconductor spintronics. The spin Hall effect refers to the generation of a pure spin current transverse to a charge current, resulting in a spontaneous spin accumulation near sample boundaries without the need for magnetic fields or materials. Recent experiments toward imaging this electrically generated spin polarization with both spatially and temporally resolved Kerr rotation microscopy in bulk zincblende semiconductors are discussed. Both current-induced in-plane spin accumulation and out-of-plane spin accumulation from the spin Hall effect are observed in ZnSe up to room temperature3. In GaAs devices, spatially resolved measurements of steady-state spin Hall accumulation and associated modeling clarify the important role of drift and diffusion in transporting spins generated at sample boundaries to the device interior4. In these typical optical experiments, electrically-generated spin accumulation is measured using steady-state techniques that do not directly observe dynamics at timescales important for device operation. Here we discuss a time- and spatially-resolved measurement of the spin Hall effect using a pulsed current to drive spin accumulation5. The dynamical processes of spin accumulation and diffusion reveal spatially-dependent nanosecond timescales comparable to the electric-field dependent spin coherence time. A time-dependent decomposition analysis reconciles the observed spatial and temporal dynamics of spin accumulation from the spin Hall effect in one coherent picture.

1. Work supported by NSF, ONR, and the Hertz Foundation.

3:06PM X3.00002 The quantum spin Hall effect and the topological magneto-electric effect . SHOUCHENG ZHANG, Stanford University — Search for topologically non-trivial states of matter has become a important goal for condensed matter physics. Recently, a new class of topological insulators has been proposed. These topological insulators have an insulating gap in the bulk, but have topologically protected edge states due to the time reversal symmetry. In two dimensions the edge states give rise to the quantum spin Hall (QSH) effect, in the absence of any external magnetic field. I shall review the theoretical prediction1 of the QSH state in HgTe/CdTe semiconductor quantum wells, and its recent experimental observation2. The QSH effect can be generalized to three dimensions as the topological magneto-electric effect (TME) of the topological insulators3. I shall also present realistic experimental proposals to observe fractional charge5, spin-charge separation and the deconfinement of the magnetic monopoles in these novel topological states of matter.


3:42PM X3.00003 Experimental observation of the quantum spin Hall state in HgTe quantum wells . LAURENS MOLENKAMP, Würzburg University — Spin-orbit interaction in semiconductors causes many interesting and potentially useful transport effects, such as e.g. the presently very topical spin-Hall effect1. So far no direct evidence for a ballistic, intrinsic SHE (i.e. resulting from the band structure) has been obtained by transport experiments. Here, we demonstrate that in specially designed nanostructures2, which are based on narrow gap HgTe type-III quantum wells, a detection of the spin signal is possible via non-local voltage measurements. Recently, it was pointed out that such HgTe quantum wells, that exhibit an inverted band structure where the ordering of electron- and hole-like states is interchanged, are topologically non-trivial insulators3, in which the quantum spin Hall insulator state4 should occur. In this novel quantum state of matter, a pair of spin polarized helical edge channels develops when the bulk of the material is insulating, leading to a quantized conductance. I will present transport data provide very direct evidence for the existence of this third quantum Hall effect: when the bulk of the material is insulating, we observe a quantized electric conductance5. Finally, we demonstrate how a combination of the techniques used in the above experiments allows us to verify that the transport in the quantum spin Hall insulator state indeed occurs through spin-polarized helical edge channels.

4:18PM X3.00004 Theory of Topological Insulators, LIANG FU, University of Pennsylvania — Topological insulators are materials with a bulk excitation gap generated by the spin orbit interaction, and which are different from conventional insulators. This distinction is characterized by $Z_2$ topological invariants, which characterize the ground state. In two dimensions a single $Z_2$ invariant describes the quantum spin Hall insulator phase. In three dimensions there are four $Z_2$ invariants, distinguishing “weak” (WTI) and “strong” (STI) topological insulators. The STI phase is characterized by the presence of unique gapless surface states whose Fermi surface encloses an odd number of 2D Dirac points. We will argue theoretically that the semiconducting alloy Bi$_{1-x}$Sb$_x$ is a strong topological insulator — a prediction that has recently been confirmed experimentally. We will next show that the proximity effect between this unique surface phase and an ordinary superconductor leads to a two dimensional state that resembles a spinless $p_+ + i p_-$ superconductor, but does not break time reversal symmetry. This state supports zero energy Majorana bound states at vortices, and may provide a new venue to realize proposals for topological quantum computing.

4:54PM X3.00005 Observation of a New Topological Phase of Quantum Matter: Quantum Hall-like Effect without Magnetic Field1. M. ZAHID HASAN, Department of Physics, Princeton University — Most quantum states of condensed-matter are categorized by the spontaneously broken symmetries. The remarkable discovery of charge quantum Hall effects (1980s) revealed that there exists an organizational principle of matter based not on the spontaneously broken symmetry but only on the topological distinctions in the presence of time-reversal symmetry breaking. In the past few years, theoretical developments suggest that new classes of topological states of matter might exist that are purely topological in nature in the sense that they do not break time-reversal symmetry hence can be realized without any applied magnetic field. Quantum Hall-like effects without magnetic field. In this presentation, I report a series of experimental results documenting and demonstrating the existence of such a topologically ordered time-reversal-invariant state of matter and discuss the exotic electromagnetic and spin properties this novel phase of quantum matter might exhibit and outline their potential use.

1“A Topological Dirac insulator in a Quantum Spin Hall Phase” Hsieh et.al., NATURE 452, 970 (2008). This work is supported by DOE, NSF and Princeton University.

Thursday, March 19, 2009 2:30PM - 5:30PM – Session X4 DPOLY: Responsive Gels at Surfaces and in the Bulk 306/307

2:30PM X4.00001 Global Signaling of Localized Impact in Chemo-responsive Gels, ANNA BALAZS, University of Pittsburgh — A vital function performed by skin is to send a chemical alarm signal throughout the system in response to irritation or damage. Using our recently developed 3D model for chemo-responsive gels, we design a coating that can perform an analogous, biomimetic function. Our system consists of a polymer gel undergoing the Belousov-Zhabotinsky (BZ) reaction. We show that such coatings respond to a spatially localized mechanical force by exhibiting a range of signaling behavior. For example, an initially stationary gel can emit transient waves in response to a sufficiently weak, localized impact. A stronger localized impact, however, can generate a global signal, which encompasses both chemical waves and surface ripples that propagate across the entire sample. This complex dynamical response persists even after the force is lifted. Furthermore, the spatial patterns formed by these oscillating gels reveal the location and magnitude of the applied force. Our findings open up the possibility of harnessing BZ gels for a range of applications, such as creating sensors that transmit a global signal in response to a local mechanical impact.

3:06PM X4.00002 Volume-Phase Transitions and Swelling Instabilities in Surface-Tethered Responsive Gels, RYAN TOOMEY, University of South Florida — Responsive polymer hydrogels have opened exciting opportunities for breathable structures that adopt to environmental cues. Such structures can be designed from a variety of chemical motifs that endow specific response behavior at the material level. Moreover, mechanically pinning a responsive gel to a surface presents further opportunities for designing specific shape-volument transitions due to swelling-induced deformations that arise within confined structures. We present a simple technique for fabricating responsive polymer networks based on copolymers comprising the photocross reactive methacryloyloxybenzophenone (MaBP). This approach permits the synthesis of photo-cross-linkable polymers that are easily patterned with thicknesses down to 80 Angstroms. Using a combination of neutron reflection, QCM- D, and ATR-FTIR, we have mapped the volume-phase behavior of ultra-thin layers of responsive networks as a function of chemical functionality, cross-link density, and thickness. Interestingly enough, neutron reflection reveals diffuse interfaces at the periphery of surface-attached networks that grow with the degree of swelling, pointing to surface fluctuations that result from biaxial compression. Finally, confocal microscopy has been used to map three-dimensional swelling in patterned structures revealing swelling instabilities from surface undulations to macroscopic buckling depending on the aspect ratio of the pattern.

3:42PM X4.00003 Supramolecular Gels in the Bulk and at Surfaces1 , STEPHEN CRAIG, Duke University — Responsive gels might be broadly classified into two groups: those in which the material response is mediated by a phase transition involving the cooperative behavior of many molecules, or molecule moieties, together, and those in which the material response is dictated by the behavior of individual molecular components acting independently of each other. This talk will discuss the properties of supramolecular gels as a representative of the latter class of responsive materials. In the context of this talk, supramolecular gels are solvent-swollen polymer networks in which the connections between polymer chains that define the network are due to specific, directional, and reversible 1:1 interactions between molecular partners. In such cases, the properties of the network are responsive to the same stimuli that influence the reversible interaction between the molecular partners. The magnitude and sensitivity of stimulus-responsiveness in supramolecular gels is greatest in the vicinity of the gel point, and the characteristics of the sol-gel phase transition will be described for a family of coordinatively cross-linked poly(4-vinylpyridine) (PVP) organogels. It will be shown that the cross-linking interaction can have profound effects on the mechanical properties of similar, surface-bound networks prepared from end-grafted PVP.

1Support from NSF CHE-0646670 is gratefully acknowledged.

4:18PM X4.00004 Photoresponsive Polymers: Converting Light to Mechanical Work, RICHARD A. VAIA, Air Force Research Laboratory — The ability to remotely control the creation of mechanical work, rapidly, with high spatial precision, and over long distances, offers many intriguing possibilities. Whether driving direct conformational changes, initiating reversible chemical reactions to release stored strain, or converting the photon to a local temperature increase, combinations of photoactive units, nanoparticles, ordered mesophases and polymeric networks are providing an expansive array of photo-responsive polymer options. By combining these material responses with kinematic concepts, mechanical devices can be demonstrated that exhibiting tunable and controllable macroscopic deformation, high-frequency oscillation or directional motion. Specifically, we will discuss recent investigation of liquid crystal polymer networks containing main chain and pendant azobenzene moieties (azo-LCN) with modulus ~1.35GPa that are actuated at the absorptive overlap of the cis and trans confirmers (442 nm). Cantilevers and unconstrained beams of these azo-LCNs can be controlled by polarization angle of the source, as well as by a specific optical exposure history (on-off), with responses ranging from lateral motion to oscillations in excess of 30Hz. These phenomena reflect an underlying interaction between the mesophase order, the network architecture and kinematic constraints of the exposed material. In collaboration with Timothy Bunning, Timothy White, Hilmar Koerner, Air Force Research Laboratory; and Nelson Tabiryan, BEAM Co.

4:54PM X4.00005 3D Microfabrication of responsive protein gels, JASON SHEAR, The University of Texas at Austin — No abstract available.
2:30PM X5.00001 Collective dynamics of rigid and deformable self-propelled particles1, ARSHAD KUD RollI, Department of Physics, Clark University, Worcester, MA 01610 — We discuss a series of experiments with granular matter with novel shapes which self-organize upon excitation. Previously, we reported experiments with rigid rod shaped particles with asymmetric mass distributions which show directed motion on a vibrated plate [1]. Recognizing that such a system is a simple physical model of self-propelled particles, we discuss the observed collective behavior such as aggregation at the boundaries and swirling motion in the context of various minimal leaderless models of active living systems such as bacterial colonies and hoofed animal herds which show self-organization. We will introduce and discuss the dynamics of deformable shapes consisting of a head and a tail composed of a bead chain which is shown to undergo directed motion because of differential friction associated with the head and the body. [1]: “Swarming and swirling in self-propelled granular rods,” A. Kudrolli, G. Lumay, D. Volfson, and L. Tsimring, Phys. Rev. Lett. 100, 058001 (2008).

3:06PM X5.00002 Three dimensional reconstruction of starling flocks: an empirical investigation of collective animal behavior, IRENE GIARDINA, CNR-INFM — Bird flocking is a striking example of animal collective behaviour: thousands of birds gather above the roosting site, forming sharp-bordered flocks, which wheel and turn with remarkable coherence and synchronization. Despite an increasing theoretical interest, empirical investigations of collective motion have been limited so far by the difficulties of getting data on large systems. By means of stereoscopic photography and using statistical mechanics, optimization theory and computer vision techniques, we have measured for the first time the three-dimensional positions and trajectories of individual birds in groups of up to three thousands elements. This allowed us to analyze global morphological properties of the flocks, as well as structural and dynamical properties. Most notably, we investigated the nature of the inter-individual interaction. We found that the interaction between birds does not depend on their mutual metric distance, as most current models and theories assume, but rather on the topological distance (number of intermediate neighbors). In fact, we discovered that each individual interacts on average with a fixed number of neighbors (six-seven), rather than with all neighbors within a fixed metric distance. We argue that a topological interaction of this kind is indispensable to maintain flock’s cohesion against the large density changes caused by external perturbations, typically predation. More recently, we characterized the velocity field, and computed dynamical observables. We showed that flocks exhibit long range correlations, which are a signature of their remarkable collective behavior.

3:42PM X5.00003 Self Propelled Particles: from microdynamics to hydrodynamics1, APARNA BASKARAN, Syracuse University — In this talk I will illustrate the derivation of a unified continuum description of the large scale collective behavior of active matter from two specific physical microscopic dynamical models: stroke-averaged swimmers moving through a viscous fluid and self-propelled hard rods moving on a substrate. New results at large scales include a lowering of the density of the isotropic-nematic transition, an enhancement of longitudinal diffusion of the self-propelled orientable units, and a strong enhancement of boundary effects in confined self-propelled systems.

4:18PM X5.00004 Active biopolymer gels: from cells to tissues1, GIJSJE KOENDERINK, FOM Institute AMOLF — Living cells are active soft materials that are far out of thermodynamic equilibrium. They continuously use up chemical energy in order to generate forces that drive processes such as cell migration and division. Moreover, cells actively remodel their surrounding extracellular matrix (primarily collagen), so whole tissues can also be regarded as active soft materials. The aim of our research is to understand the physical mechanisms underlying the self-organization and mechanics of cells and tissues. To this end we use an experimental approach and study simplified model systems for the cytoskeleton (purified actin, tubulin, and accessory proteins) and for tissues (fibroblast-populated collagen and fibrin gels). We use microscopy and rheology to investigate the structure and mechanics on different length scales, from the single protein up to macroscopic level. I will discuss two examples of active mechanical behavior, namely in purified actin-myosin networks, and in purified fibrin matrices embedded with contractile fibroblasts. In both cases we observe active contraction and active stiffening. We quantify the active forces and examine how the structure and mechanics of the active gels depend on motor/cell density.

4:54PM X5.00005 Beller Lectureship Talk: Active response of biological cells to mechanical stress, SAMUEL SAFFRAN, Dept. Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel 76100 — Forces exerted by and on adherent cells are important for many physiological processes such as wound healing and tissue formation. In addition, recent experiments have shown that stem cell differentiation is controlled, at least in part, by the elasticity of the surrounding matrix. We present a simple and generic theoretical model for the active response of biological cells to mechanical stress. The theory includes cell activity and mechanical forces as well as random forces as factors that determine the polarizability that relates cell orientation to stress. This allows us to explain the puzzling observation of parallel (or sometimes random) alignment of cells for static and quasi-static stresses and of nearly perpendicular alignment for dynamically varying stresses. In addition, we predict the response of the cellular orientation to a sinusoidally varying applied stress as a function of frequency and compare the theory with recent experiments. The dependence of the cell orientation angle on the Poisson ratio of the surrounding material distinguishes cells whose activity is controlled by stress from those controlled by strain. We have extended the theory to generalize the treatment of elastic inclusions in solids to "living" inclusions (cells) whose active polarizability, analogous to the polarizability of non-living matter, results in the feedback of cellular forces that develop in response to matrix stresses. We use this to explain recent observations of the non-monotonic dependence of stress-fiber polarization in stem cells on matrix rigidity. These findings provide a mechanical correlate for the existence of an optimal substrate elasticity for cell differentiation and function.

1This work was done in collaboration with M. Cristina Marchetti, with support of NSF grants DMR-0705105 and DMR-0806511.

2Supported by NSF-DMR 0605664

Thursday, March 19, 2009 2:30PM - 5:30PM —
Session X5 GSNP: Active Soft Matter: From Granular Rods to Flocks to Living Cells 401/402

Thursday, March 19, 2009 2:30PM - 5:30PM —
Session X6 DCOMP: Rahman Prize Lecture and Theory of Multiferroics 406
in vivo extrinsic and intrinsic nucleosome positioning signals. In order to see the relative importance of such signals for nucleosome positioning, currently available bioinformatics methods for predicting nucleosome positions are trained on sequence data and are thus unable to distinguish between long-range interactions. Hence, much of what we know about spin glasses and related systems comes from numerical simulations on simplified models. In this talk I will describe some of the challenges in performing reliable spin glass simulations. Then I will discuss several questions concerning phase transitions in spin glasses and related systems that have been addressed by simulations in recent years including (i) whether there is universality, (ii) whether there is a "vortex glass" transition in a disordered type-II superconductor in a magnetic field, (iii) whether "chiralities" play a crucial role in Heisenberg spin glasses, and (iv) whether there is a line of transitions (AT line) in a magnetic field.

3:06PM X6.00002 Superexchange-driven Magnetoelectricity in Magnetic Vortices, KRIS DELANEY, UCSC — We demonstrate that spins in topologically frustrated antiferromagnetic systems can form periodic arrays of magnetic vortices with symmetry allowing for a linear magnetoelectric response. Realization of this magnetic structure can be provided by transition-metal oxides with a layered Kagomé lattice. In such systems, an appropriately structured lattice leads to a microscopic coupling between spins and polar lattice distortions via Anderson superexchange, which has the potential to provide a large magnetoelectric response. In order to quantitatively probe the strength of the magnetoelectric coupling, we have performed density functional theory calculations in the presence of an applied electric field (using linear response) for hexagonal manganites. We demonstrate that the coupling is large and summarize the challenges for achieving such a response in real materials.

3:42PM X6.00003 First-Principles Approach to Lattice-Mediated Magnetoelectric Effects¹, JORGE IFÍGUEZ, Institut de Ciencia de Materiales de Barcelona (CSIC) — I will present a microscopic theory of the magnetoelectric response of an insulator, and derive from it an analytical expression for the lattice-mediated part of the effect. As I will show, such a result provides us with distinct hints at strategies to increase the magnitude of the response, as well as with a convenient method for performing first-principles calculations. I will illustrate the usefulness of the proposed approach with applications to Cr₂O₃, a model magnetoelectric crystal, and BiFeO₃ and related compounds, the best studied, and arguably most technologically promising, family of multiferroics. Ref.: J. Ifiguez, Phys. Rev. Lett. 111, 117201 (2008).

1Work funded by FP6-STRREP MaCoMuFi.

4:18PM X6.00004 First-principles Study of Improper Ferroelectricity in TbMnO₃, ANDREI MALASHYEVICh, Rutgers University — Perovskite TbMnO₃ at room temperature forms an orthorhombically distorted lattice with the Pnma space group. Below ~27 K the magnetic moments on the Mn atoms adopt an incommensurate cycloidal wave order, and simultaneously a polarization appears along the c direction. We present the results of our first-principles theoretical study of the magnetically induced polarization in TbMnO₃ with a commensurate cycloidal wave of Mn³⁺ moments with a wave-vector close to the experimental value.¹ The calculations are based on density-functional theory in the local-density approximation with the on-site Coulomb correction (LDA+U). The polarization is computed using the Berry-phase technique. We show, in particular, that the spin-orbit interaction is essential for the magnetoelectric coupling. We compute both the electronic and the lattice-mediated contributions to the polarization, and find that the latter is strongly dominant. We analyze the spin-orbit induced forces and lattice displacements from both atomic and mode-decomposition viewpoints, and show that a simple model based on nearest Mn-Mn neighbor Dzyaloshinskii-Moriya interactions is not able to account fully for the results. The direction and magnitude of our computed polarization are in good agreement with experiment. If time permits, calculations on other magnetically induced improper ferroelectrics will be discussed.

1Work supported by NSF grant DMR-0549198


4:54PM X6.00005 Density functional study of the spin exchange interactions, magnetic structures, and ferroelectric polarizations of multiferroics driven by magnetic order, MIKE WHANGBO, North Carolina State University — The electronic structures of magnetic insulators LiCuVO₄, LiCuO₂, TbMnO₃, Ca₃CoMnO₇, MnWO₄, CuFeO₂, Ba₂CoGe₂O₇ and CuBr were examined on the basis of first principles DFT+U+SOC calculations to evaluate their spin exchange parameters and account for their ordered magnetic structures. We then explored how the electric polarizations of these compounds are related to the magnetic ordering and spin-orbit coupling. In this talk results of our studies will be presented.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X7 DBP: DNA Loop Formation, Nucleosome Positioning and Transcriptional Regulation

2:30PM X7.00001 Statistical mechanics of chromatin: Inferring free energies of nucleosome formation from high-throughput data sets¹, ALEXANDRE MOROZOv, Department of Physics & Astronomy, Rutgers University — Formation of nucleosome core particles is a first step towards packaging genomic DNA into chromosomes in living cells. Nucleosomes are formed by wrapping 147 base pairs of DNA around a spool of eight histone proteins. It is reasonable to assume that formation of single nucleosomes in vitro is determined by DNA sequence alone: it costs less elastic energy to wrap a flexible DNA polymer around the histone octamer, and more if the polymer is rigid. However, it is unclear to which extent this effect is important in living cells. Cells have evolved chromatin remodeling enzymes that expend ATP to actively reposition nucleosomes. In addition, nucleosome positioning on long DNA sequences is affected by steric exclusion — many nucleosomes have to form simultaneously without overlap. Currently available bioinformatics methods for predicting nucleosome positions are trained on in vivo data sets and are thus unable to distinguish between extrinsic and intrinsic nucleosome positioning signals. In order to see the relative importance of such signals for nucleosome positioning in vivo, we have developed a model based on a large collection of DNA sequences from nucleosomes reconstituted in vitro by salt dialysis. We have used these data to infer the free energy of nucleosome formation at each position along the genome. The method uses an exact result from the statistical mechanics of classical 1D fluids to infer the free energy landscape from nucleosome occupancy. We will discuss the degree to which in vitro nucleosome occupancy profiles are predictive of in vivo nucleosome positions, and will estimate how many nucleosomes are sequence-specific and how many are positioned purely by steric exclusion. Our approach to nucleosome energetics should be applicable across multiple organisms and genomic regions.

1AM acknowledges financial support from the BioMaPS Institute for Quantitative Biology.

3:06PM X7.00002 to be determined by you, LAURA FINZI, Emory University — No abstract available.
3:42PM X7.00003 Interconvertible Lac Repressor–DNA Loops Revealed by Single-Molecule Experiments, MARTIN GUTHOLD, Wake Forest University — At many promoters, transcription is regulated by simultaneous binding of a protein to multiple sites on DNA, but the structures and dynamics of such transcription factor-mediated DNA loops are poorly understood. We directly examined in vitro loop formation mediated by E. coli lactose repressor using single-molecule structural and kinetics methods. Small (150 bp) loops form quickly and stably, even with out-of-phase operator spacings. Unexpectedly, repeated spontaneous transitions between two distinct loop structures were observed in individual protein–DNA complexes. The results imply a dynamic equilibrium between a novel loop structure with the repressor in its crystallographic “V” conformation and a second structure with a more extended linear repressor conformation that substantially lessens the DNA bending strain. The ability to switch between different loop structures may help to explain how robust transcription regulation is maintained even though the mechanical work required to form a loop may change substantially with metabolic conditions.

4:18PM X7.00004 The Energy Landscape of Hyperstable LacI-DNA Loops, JASON KAHN, Chem. and Biochem., Univ. Maryland College Park — The Escherichia coli LacI protein represses transcription of the lac operon by blocking access to the promoter through binding at a promoter-proximal DNA operator. The affinity of tetrameric LacI (and therefore the repression efficiency) is enhanced by simultaneous binding to an auxiliary operator, forming a DNA loop. Hyperstable LacI-DNA loops were previously shown to be formed on DNA constructs that include a sequence-directed bend flanked by operators. Biochemical experiments showed that two such constructs (9C14 and 11C12) with different helical phasing between the operators and the DNA bend form different DNA loop shapes. The geometry and topology of the loops and the relevance of alternative conformations suggested by probable flexible linkers in LacI remain unclear. Bulk and single molecule fluorescence resonance energy transfer (SM-FRET, with D. English) experiments on a dual fluorophore-labeled 9C14-LacI loop demonstrate that it adopts a single, stable, rigid closed-form loop conformation. Here, we characterize the LacI-9C14 loop by SM-FRET as a function of inducer isopropyl-β-D-thiogalactoside (IPTG) concentration. Energy transfer measurements reveal partial but incomplete destabilization of loop formation by IPTG. Surprisingly, there is no change in the energy transfer efficiency of the remaining looped population. Models for the regulation of the lac operon often assume complete disruption of LacI-operator complexes upon inducer binding to LacI. Our work shows that even at saturating IPTG there is still a significant amount of LacI-DNA complexes in a looped state, in accord with previous in vivo experiments that show incomplete induction (with J. Maher). Finally, we will report progress on characterizing the “energy landscape” for DNA loop switching upon systematic variation of the DNA linkers between the operators and the bending locus. Rod mechanics simulations (with N. Perkins) provide testable predictions on loop stability, topology, and FRET.

4:54PM X7.00005 Mechanics of Protein-Mediated DNA Looping, JENS-CHRISTIAN MEINERS, University of Michigan — The formation of looped DNA-protein complexes in which a protein or protein assembly binds to multiple distant operator sites on the DNA is a common feature for many regulatory schemes on the transcriptional level. In a living cell, a multitude of mechanical forces and constraints act on these complexes, and it is imperative to understand their effects on biological function. For this aim, we study the lactose repressor as a model system for protein-mediated DNA looping in single-molecule experiments. Using a novel axial constant-force optical trapping scheme that allows us to manipulate sub-micron DNA fragments with well-controlled forces down to the 10 fN range, we show that mechanical tension in the substrate DNA of hundred femtonewton is sufficient to disrupt the loop formation process, which suggests that such mechanical tension may provide a mechanical pathway to controlling gene expression in vivo. From the force sensitivity of the loop formation process, we can also infer the topology of the looped complex; in our case an antiparallel conformation. In addition, we will present new tethered-particle microscopy data that shows lifetimes of the looped complexes that are two to three orders of magnitude shorter than those measured in biochemical competition assays and discuss possible interpretations, including the suggestion that operator binding of the lactose repressor tetramer leads to a destabilization of the dimer-dimer interface and that thus the loop breakdown process is mostly a dissociation of the tetramer into two dimers, instead, as widely assumed, an unbinding of the tetramer from the DNA.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X8 FHP: 50 Years of Anderson Localization 414/415

2:30PM X8.00001 Anderson localization in the seventies and beyond, DAVID THOULESS, University of Washington — Little attention was paid to Anderson’s challenging paper on localization for the first ten years, but from 1969 onwards it generated a lot of interest. Around that time a number of challenging questions were raised by the community, on matters such as the existence of a sharp distinction between localized and extended states, or between conductors and insulators. For some of these questions the answers are unambiguous. There certainly are energy ranges in which states are exponentially localized, in the presence of a static disordered potential. In a one-dimensionnal potential all states are localized. There is clear evidence, in three dimensions, for energy ranges in which states are extended and diffusive. Magnetic and spin-dependent interactions play an important part in reducing localization effects. For massive particles like electrons and atoms the lowest energy states are localized, but for massless particles like photons and acoustic phonons the lowest energy states are extended. In a one-dimensional disordered system all states are localized. Uncertainties remain. Scaling theory shows that in two-dimensional systems all states are weakly localized, and that there is no minimum metallic conductivity. The interplay between disorder and mutual interactions is still an area of uncertainty, which is very important for electronic systems. Optical and dilute atomic systems provide experimental tests which allow interaction to be much less important. The quantum Hall effect provided a system where states on the Fermi surface are localized, but non-dissipative currents flow in response to an electric field.

3:06PM X8.00002 Tests of Localization in Metals and Semiconductors, ROBERT DYNES, University of California San Diego — The metal-Insulator transition has been a subject of study for decades. It is now well known that entering the critical region of the transition the characteristics of a highly correlated system dominate. The dimensionality of the system is also very important. In this talk I will reminisce about the concepts and experiments to test models, explore systems, and investigate the role of dimensionality. Mott’s concept of a minimum metallic conductivity drove my own thinking until the landmark paper of Abrahams, Anderson, Licciardello and Ramankrishnan. A series of careful experiments testing the notions of weak localization followed this paper and provided critical tests of the concept. I will describe some of those experiments and the things we learned from this work.

3:42PM X8.00003 Anderson Localization of Light, MORDECHAI SEGEV, Technion - Israel Institute of Technology — Photonic lattices are excellent model systems for studying wave localization due to disorder. The recent progress on Anderson Localization of light will be reviewed, including the additional effects of nonlinearity, with an emphasis on the universal features common to all wave systems in nature.

4:18PM X8.00004 Anderson Localization and Mesoscopics, IGOR LERNER, University of Birmingham, B15 2TT, United Kingdom — I will review certain trends developed within the last thirty years of research on Anderson Localization with emphasis on the description of the Anderson transition in terms of the entire distribution function of the conductance mesoscopic fluctuations, and on the role of electron-electron interactions.
4:54PM X8.00005 Direct observation of Anderson localization of matter-waves in an optical disorder1, ALAIN ASPECT, Institut d’Optique and CNRS — In 1958, P.W. Anderson predicted the localization1 of electronic wave functions in disordered crystals, and the resulting absence of diffusion. It has been realized later that Anderson Localization is ubiquitous in wave physics2, and this has prompted an intense activity to observe it with light, microwaves, sound waves, and electron gases, but to our knowledge there was no direct observation of exponential spatial localization of matter-waves (electrons or others). We have observed directly3 exponential localization of the wave function of ultracold atoms released into a one-dimensional waveguide in the presence of a controlled disorder created by laser speckle. We will present this work, and the prospects of extending that experimental scheme to quantum gases in higher dimensions (2D and 3D), and with controlled interactions. We will also discuss its significance in the rapidly growing field of quantum simulators.

1 Supported by CNRS and by the “programme blanc” of the Agence Nationale de la Recherche.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X9 GSNP: Focus Session: Jamming: Theory and Experiment II 303

2:30PM X9.00001 Jamming in Vibrated Granular Systems1, BRIAN UTTER, James Madison University — Granular materials exist all around us, from avalanches in nature to the mixing of pharmaceuticals, yet the behavior of these “fluids” is poorly understood. Their flow can be characterized by the continuous forming and breaking of a strong force network resisting flow. This jamming/unjamming behavior is typical of a variety of systems, including granular flows, and is influenced by factors such as grain packing fraction, applied shear stress, and the random kinetic energy of the particles. I’ll present experiments on quasi-static shear and free-surface granular flows under the influence of external vibrations. By using photoelastic grains, we are able to measure both particle trajectories and the local force network in these 2D flows. We find through particle tracking that dense granular flow is composed of comparable contributions from the mean flow, affine, and non-affine deformations. During shear, sufficient external vibration weakens the strong force network and reduces the amount of flow driven by interfaces. In a rotating drum geometry, large vibrations induce failure as might be expected, while small vibration leads to strengthening of the pile. The avalanching behavior is also strongly history dependent, as evident when the rotating drum is driven in an oscillatory motion, and we find that sufficient vibration erases the memory of the pile. These results point to the central role of the mobilization of friction in quasi-static granular flow.

1 Supported by NSF REU DMR-0353773 and Research Corporation CC-7260.

3:06PM X9.00002 Scaling of Foam Flows near Jamming, MARTIN VAN HECKE, ERIK WOLDHUIS, BRIAN TIGHE, Leiden University, JORIS REMMERS, Eindhoven University, WIM VAN SAARLOOS, Leiden University — We probe the scaling behavior of flows near the jamming transition of soft, viscous discs in a variant of the well known bubble-model for foams, where we assume that the viscous forces between contacting bubbles scale with the relative velocity with an adjustable exponent α. This allows us to explore the non-trivial dependence of global flow exponents on the local exponent α. Even though we find that elastic stresses dominate the global stresses in the system, the exponent α which governs the sub-dominant viscous interactions still sets the global scaling exponents.

3:18PM X9.00003 ABSTRACT WITHDRAWN —

3:30PM X9.00004 Rheology of Soft Suspensions near Jamming1, KERSTIN NORDSTROM, EMLIE VERNEUIL, PAULO ARRATIA, University of Pennsylvania, JERRY GOLLUB, Haverford College, DOUGLAS DURIAN, University of Pennsylvania — The rheology of a suspension of soft colloidal particles is investigated using a pressure-driven flow in a deep 25 μm wide microchannel. The system is composed of N-isopropylacrylamide (NIPA) colloidal microgel particles, suspended in aqueous solution. NIPA is temperature-sensitive in that the hydrodynamic radius decreases rapidly with an adjustable exponent

α

. The largest event and number of events increase roughly linearly with the system width L for L varying from 25 to 400 particle diameters. Increasing

α


1 Supported by NSF MRSEC /DMR05-20020.

3:42PM X9.00005 Inertia and the Distribution of Avalanches in Sheared Glasses, KENNETH SALERNO, MARK ROBBINS, Johns Hopkins University, CRAIG MALONEY, Carnegie Mellon University — Many slowly driven condensed matter systems show highly intermittent and spatially organized dynamics where relaxation proceeds via “avalanches”. This talk describes the role of inertia in determining the distribution of avalanches in sheared glassy systems. Simulations were performed on binary mixtures of Lennard-Jones particles in two dimensions. The distribution of

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isopropylacrylamide (NIPA) colloidal microgel particles, suspended in aqueous solution. NIPA is temperature-sensitive in that the hydrodynamic radius decreases

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3:54PM X9.00006 Density of states in two-dimensional colloidal system, KE CHEN, ZEXIN ZHANG, PETER YUNKER, ARJUN YODH, Department of Physics and Astronomy, University of Pennsylvania — The vibrational density of states (VDOS) of particles in a two-dimensional binary colloidal system was investigated using video microscopy. Our ultimate goal is to explore how the VDOS varies near the jamming transition [1]. Various distributions of NIPA particles, whose diameters can be tuned by small temperature variations, were loaded into parallel-plate microscope cells, and their motions tracked with video microscopy. This approach permits in-situ observation over a wide range of particle packing fractions, from colloidal fluids to colloidal glasses. A search for excess VDOS at low frequencies in colloidal glass is ongoing. 1. N. Xu, M. Wyart, A. J. Liu, and S. R. Nagel, Phys. Rev. Lett. 98, 175502 (2007) This work is supported by NSF DMR-080488, MRSEC DMR-0520020.
4:06PM X9.00007 Applying the model of Soft Glassy Rheology to slowly driven dense granular matter\(^1\), DAPENG BI, BULBUL CHAKRABORTY, Brandeis University — In recent work by S. Henkes and B. Chakraborty (PRL 95, 198002 (2005)), a new statistical framework is proposed to describe static granular packings. In this framework, stress replaces energy as the conserved quantity and fluctuations in the stress are controlled by a quantity analogous to the thermodynamic temperature. We adapt this framework in the quasi-static limit and the model of Soft Glassy Rheology (P. Sollich, PRE 78, 2020 (1997)) to describe the rheological behavior of slowly driven dense granular matter. The model explains the experimental observation of R. P. Behringer et al. (Nature 421, 928 (2003)). We will describe ongoing efforts to apply this model to different scales of slowly driven granular media, and to relate the model to critical dynamics in other driven random media.

\(^1\)Work supported by NSF-DMR 0549762

4:18PM X9.00008 Theory of random packings, HERNAN MAKSE, City College of New York, CHAOMING SONG, PING WANG — We present a theory of random packings to describe the statistical mechanics of jammed matter with the aim of shedding light to the long-standing problem of order and long-range correlations in random jammed packings. We present a new statistical framework where state relations are determined by a conserved stress and fluctuations in the stress. We will compare our results to a number of systems for which we have high-quality measurements of their static and dynamical properties.

4:30PM X9.00009 Dense packings of hard tetrahedra, AMIR HAJI AKBAR, University of Michigan, Ann Arbor, XIAOYU ZHENG, Kent State University, ROLFE PETSCHER, Case Western Reserve University, PETER PALFFY-MUHORAY, Kent State University, SHARON GLOTZER, University of Michigan, Ann Arbor — The densest packing of tetrahedra remains an unsolved problem, and there has been much recent debate. We simulate dense packings of mathematically smooth, hard regular tetrahedra using NPT Monte Carlo simulations and determine the density-pressure equation of state. We find disordered packings with densities that significantly exceed the hard-sphere FCC packing density of 0.74084090. Our findings thus demonstrate that tetrahedra obey Ulam’s conjecture that spheres pack with a lower maximum packing density than any other hard convex object, despite recent conjecture to the contrary. The dense packings that we have found do not seem to be crystalline but are instead dense random packings. We show that the system is able to achieve such high packing densities by the local ordering of tetrahedra into certain favorable motifs, forming larger structures that pack efficiently but are overall jammed. We speculate that one or several denser crystalline packings exist.

4:42PM X9.00010 ABSTRACT WITHDRAWN

4:54PM X9.00011 Continuous Geometric Families of Mechanically Stable Particle Packings, GUOJIE GAO, Dept. of Mechanical Engineering, Yale University, JERZY BLAWZDZIEWICZ, COREY O’HERN, Dept. of Mechanical Engineering & Dept. of Physics, Yale University — We have performed numerical simulations of quasi-static shear flow of soft disks at zero pressure to generate mechanically stable (MS) packings as a function of applied shear stress/strain in small 2D systems ranging from 4 to 20 disks. In systems composed of frictionless disks, we find that at any given shear strain, there are a finite number of discrete MS packings characterized by the positions of all particles. In contrast, there are an infinite number of MS packings during continuous shear flow that form a finite geometric families (characterized by the network of interparticle contacts) as a function of shear strain. We count the number of geometric families and measure their length in strain as a function of system size. In particular, we will determine whether the MS packings at finite shear have different structural and mechanical properties from those at zero shear. We also study the effects of friction on MS particle packings. In contrast to frictionless MS packings, frictional packings form continuous geometric families even at a zero shear strain.

5:06PM X9.00012 Mechanically Stable Packings of Spherocylinders\(^1\), TIMOTHY GREEN, SCOTT FRANKLIN, RIT — Piles of long, thin rods are substantially more stable to perturbations than those of ordinary sand or rice. We generate 3d mechanically stable packings of spherocylinders by alternately enlarging particles (with an elastic repulsive interaction) and using a conjugate gradient minimization of the total elastic energy. The minimum stable packing is defined as the least dense packing for which the minimum energy is non-zero, and we investigate the average contact number, the spectrum of vibrational modes in the dynamical matrix, and other properties of this critical packing. We also test whether spherocylinders obey the isostatic conjecture, which states that the average contact number at ϕc is twice the number of degrees of freedom (for spherocylinders, 5). Spherocylinders’ straight edges, compared with the convex sides of ellipsoids, puts the isostatic conjecture in jeopardy, perhaps requiring a greater number of contacts to maintain stability.

\(^1\)Funded with support from the National Science Foundation (DMR-0706353)

5:18PM X9.00013 On the study of force-balance percolation, J. M. SCHWARZ, Syracuse University, M. JENG, Microsoft Corporation — We study models of percolation where there are constraints on the occupation of sites that mimic force-balance, i.e. for a site to be stable (remain occupied) requires occupied neighboring sites in all four compass directions in two dimensions. We prove rigorously that ϕc < 1 for the two-dimensional models studied. Numerical data indicate that the force-balance percolation transition is discontinuous with a growing crossover length, and the two-dimensional percolation model, but with the same underlying mechanisms causing the transition in both cases. In other words, force-balance percolation and jamming percolation may indeed belong to the same universality class. We find a lower bound for the correlation length in the connected phase and that the correlation function does not appear to be a power law at the transition. Finally, we study the dynamics of the culling procedure invoked to obtain the force-balance configurations and measure a dynamical exponent similar to that found in sandpile models.

Thursday, March 19, 2009 2:30PM - 5:18PM —
Session X10 DCMP: Insulators and Dielectrics: Defects, Structure, and Mechanical and Dynamical Properties 304

2:30PM X10.00001 Dynamics of implant damage as a precursor to nanocrystal nucleation, MATTHEW J. BECK, SOKRATES T. PANTELIDES, Vanderbilt University — Ion implantation into a-SiO\(_2\) leads to the self-assembly of metal or semiconductor nanocrystal arrays having applications in optical and non-volatile memory devices. The production of uniform arrays of similarly-sized nanocrystals within the a-SiO\(_2\) matrix has been shown to depend strongly on nucleation conditions. Here we report results of quantum mechanical calculations probing the atomic-scale dynamics in the first few nanoseconds following low-energy (RCP) and high-energy (RLP) implantation. We show that low-energy (with KE<100 eV) implants produce individual, isolated defects in the a-SiO\(_2\) structure, but rather produce nanoscale defect pockets. These defect pockets are sources for oxygen out-diffusion, and subsequently represent seed regions for nanocrystal nucleation.
JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The development of gate-stack structures for novel CMOS applications has

2:42PM X10.00002 Optical Emission from F2 (CN−) centers in CsCl1 JOSEPH WEST, Indiana State University, RICHARD DALLINGER, Wabash College, RYAN LIDSTER, Indiana State University — Strong, previously unreported, emission from at least two different excited electronic states of F2 (CN−) centers in CsCl has been measured following excitation at 532 nm, 514 nm and 568 nm. The temperature dependence of emission at 532 nm was obtained over the temperature range of 16K through 160K. No emission under excitation at 633 nm was detected. The presence of emission following excitation at the higher energies, but absent under 633 nm excitation, may suggest that the well-known energy transfer process from the electronic excited F-center states to the vibrational CN− energy levels in this system occurs from a single common relaxed excited electronic state associated with the absorption band at 633 nm.

1 Prepared by LLNL under Contract DE-AC52-07NA27344

2:54PM X10.00003 Ab-Initio investigation of defects in GaTe1, CEDRIC ROCHA LEAO, VINCENZO LORDI, Lawrence Livermore National Lab — Materials that are good candidates for room-temperature radiation detectors should ideally possess several characteristics that are somewhat contradictory. A higher mobility-lifetime product is required to maximize the collection of radiation generated charge, but a relatively large bandgap is desired to minimize thermal noise. High resistivity is usually also desired, to reduce background current which degrades the detection resolution. Furthermore, a high average atomic number increases absorption of high energy radiation. GaTe is attracting recent attention for the potential to satisfy many of these criteria, but its properties are still poorly understood. Like other III-VI compounds, GaTe is a layered material, but its unusual anisotropy in the atomic planes results in rather unique mechanical and electronic properties. In this talk, we discuss ab-initio calculations of the transport properties of GaTe with respect to its application to radiation detectors. Guided by very recent experimental results, we analyze the occurrence of native defects in this materials and possible compensating extrinsic defects, and their effects on the transport properties.

3:06PM X10.00004 Electronic properties of oxygen vacancy in HfO2 within GW calculations . EUN-AE CHOI, KEE JOO CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejon 305-701, Korea — Hafnia (HfO2) has attracted much attention as a high-k dielectric material, which substitutes for silicon gate oxide in nanoscale metal-oxide-semiconductor (MOS) devices. However, there remain several problems to be resolved in hafnia-based devices, such as flat band shift and threshold voltage instability. Oxygen vacancy, as the most common intrinsic defect, is regarded as a major cause of these problems. As previous calculations mostly rely on the local-density-functional approximation (LDA), the defect levels of oxygen vacancy are not accurately determined because of the LDA band gap problem. Here we perform GW calculations for the defect levels of oxygen vacancy in monoclinic HfO2. Our calculations show that the Fermi level pinning of p+-poly Si gate electrode is due to the change from oxygen vacancy to the electrode. In addition, the charge trap of oxygen vacancy can lead to the threshold voltage instability in both nMOS and pMOS devices. Finally, we suggest that oxygen vacancy may be a cause of the gate leakage current by the Poole-Frenkel conduction.

3:18PM X10.00005 DFT Energetics of Noble Gas Impurities and Schottky Defects in UO2 . ALEXANDER THOMPSON, CHRIS WOLVERTON, Northwestern University Materials Science and Engineering, RADIATION DAMAGE IN NUCLEAR FUEL FOR ADVANCED FUSION REACTORS. The choice of the k-Al2O3 phase is based on the similarity of its density to that of amorphous Al2O3. We analyze native point defects such as vacancies, self-interstitials, and antisites, as well as various relevant impurities. Our first-principles calculations are based on density functional theory (DFT). Hybrid functionals were utilized as a means of overcoming the band-gap problem. This approach allows us to accurately assess the positions of defect levels. We use calculated band offsets to make predictions about the location of these defect levels with respect to the band gap of relevant semiconductors used as channel materials. We will discuss which defects may impede the optimal performance of devices.

3:30PM X10.00006 Polarization Patterns In GeTe From Bulk To Ferroelectric Nanoclusters . ENGIN DURGUN, University of Liege, RIAD SHALTAF, XAVIER GONZE, University of Catholic Louvain, PHILIPPE GHOSEZ, JEAN-YVES RATY, University of Liege — In this study, we investigated the ferroelectric and structural properties of GeTe crystal and nanoclusters, an alternative type of ferroelectric material, up to 1500 atoms from first-principles calculations based on density functional theory (DFT). Firstly, the dynamical, dielectric and elastic properties of GeTe in ferroelectric phase have been investigated [1]. Next, we demonstrate, for the first time at the DFT level, the existence in the interior of sufficiently large dots of polarization vortices giving rise to a net and reversible toroidal moment of polarization (G) [2]. The amplitude of G decreases with the size of the system and is only slightly suppressed due to strain relief. (iv) For Ar, Kr, and Xe, the binding energy of a noble gas impurity with the SD is larger than the energy required to form a SD, thereby providing a strong favorable binding, due to the presence of emission following excitation at the higher energies, but absent under 633 nm excitation, may suggest that the well-known energy transfer process from the electronic excited F-center states to the vibrational CN− energy levels in this system occurs from a single common relaxed excited electronic state associated with the absorption band at 633 nm.

3:42PM X10.00007 First-principles study of point defects in k-Al2O3 . JUSTIN R. WEBER, ANDREW JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The development of gate-stack structures for novel CMOS applications has stimulated interest in point defects that may occur in oxide dielectrics. We consider Al2O3 as a possible gate-stack material, and study defects in the low symmetry k-Al2O3 phase. The choice of the k-Al2O3 phase is based on the similarity of its density to that of amorphous Al2O3. We analyze native point defects such as vacancies, self-interstitials, and antisites, as well as various relevant impurities. Our first-principles calculations are based on density functional theory (DFT). Hybrid functionals were utilized as a means of overcoming the band-gap problem. This approach allows us to accurately assess the positions of defect levels. We use calculated band offsets to make predictions about the location of these defect levels with respect to the band gap of relevant semiconductors used as channel materials. We will discuss which defects may impede the optimal performance of devices.

3:54PM X10.00008 First-principles study on the electromigration of oxygen vacancy in metal oxides . SANG HO JEON, WON-JOON SON, BAE HO PARK, SEUNGWU HAN, DEPARTMENT OF PHYSICS, KONKUK UNIVERSITY TEAM, — The oxygen vacancy, which is a fundamental defect in oxides, plays a critical role in defining many electrical properties of oxides ranging from ionic conductivities to leakage behaviors. As such, to control the density and spatial distribution of the oxygen vacancy has often been an important goal in many researches on electronic devices, particularly for high-density devices, such as resistance-change random access memories (ReRAM). Despite its importance, the electromigration of oxygen vacancy has not been studied much from the microscopic point of view. In this presentation, we studied on the migration of the oxygen vacancy in metal oxides, such as MgO and TiO2. First, using the nudged elastic band (NEB) method, we estimated the migration barrier of charged oxygen vacancy under an external field. Then, we calculate the zone-center phonon modes of the bulk system to obtain the attempt frequency of the vacancy diffusion. Based on these results, we estimated the migration time of oxygen vacancy in metal oxide by using harmonic transition state theory, and it was in good agreement with the result of molecular dynamics (MD) calculation.
First-principles calculations of Ce activation in RE$_2$M$_2$O$_7$ (RE = La, Y; M = Ti, Zr, Hf). Anurag Chaudhry, Andrew Canning, Rostyslav Boutchkov, Stephen Derenzo, Niels Gronbech-Jensen — First-principles electronic structure calculations of Ce-doped La and Y compounds with composition RE$_2$M$_2$O$_7$ (RE = La, Y; M = Ti, Zr, Hf) are performed using the pseudopotential method based on the local density approximation in density functional theory. The positions of the 4f states relative to the valence band maximum and the position of the lowest 5d excited state relative to the conduction band minimum of the host material are determined. The prediction of Ce activation is based on the following criteria: (1) The energy difference between the occupied Ce 5d excited state (Ce$^{3+}$*) and the host material conduction band minimum (CBM) and (2) the degree of localization of the (Ce$^{3+}$*) excited state on the Ce atom. Our theoretical investigations indicate that Ce activation is not possible in these host materials.

Research supported by the U.S. Department of Homeland Security and by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Electric Field Induced Sub-Microsecond Resistive Switching, Nilanjan Das, Stephen Tsui, Ya-Qi Wang, Yuyi Xue, Ching-Wu Paul Chu, University of Houston — Electric field induced resistive switching in metal-oxide interfaces has attracted extensive recent interest. While many agree that lattice defects play a key role, details of the physical processes are far from clear. There is debate, for example, regarding whether the electromigration of pre-existing point defects or the field-created larger lattice-defects dominates the switch. We investigate several Ag-Pr$_{0.7}$Ca$_{0.3}$MnO$_3$ (PCMO) samples exhibiting either sub-microsecond fast switching or slow quasi-static DC switching. It is found that the carrier trapping potentials are very different for the pre-existing point defects associated with doping (and/or electromigration) and the defects responsible for the sub-μs fast-switching. Creation/removal of the defects with more severe lattice-distortions and spatial spreading (trapping potential $> 0.35$ eV), therefore, should be the dominating mechanism during sub-μs switching. On the other hand, the shallow defects (trapping potential $< < 0.2$ eV) associated with doping/annealing are most likely responsible for the resistance hysteresis (slow switch) during quasistatic voltage sweep.

Temperature dependence of Gigahertz-Range Ultra-High Frequency Micromechanical Resonators, Josef-Stefan Wenzler, Tyler Dunn, Diego Guerra, Pritiraj Mohanty — We report measurements of bulk mode resonators in the ultrahigh frequency range up to 4 GHz. The devices are fabricated with a stack of materials and actuated using piezoelectric technique. Typical dimensions of these resonators are 100 μm in length and width and 10 μm in thickness. The temperature dependence of mode frequencies and quality factor Q are investigated for temperatures ranging from 0.3 K – 400 K.

Temperature dependence of mechanical stiffness and dissipation in ultrananocrystalline diamond resonators, Vivekananda Adiga, University of Pennsylvania, Anirudha Sumant, Argonne National Laboratory, Sampa Suresh, Chris Guedmam, Innovative Micro Technology, Orlando Aucellio, Argonne National Laboratory, John Carlisle, Advanced Diamond Technologies, Robert Carpick, University of Pennsylvania — We have studied the mechanical softening and dissipation of ultrananocrystalline diamond (UNCD) resonators with temperature. Resonant excitation and ring down measurements were conducted under ultra high vacuum (UHV) conditions in a decoupled UHV atomic force microscope (AFM) to determine the Young’s Modulus and quality factor (Q) in UNCD cantilever structures. The temperature dependence of Young’s modulus revealed the characteristic Wachtman’s empirical relation. From this measurement the Debye temperature was estimated to be $\sim 1460$ K, significantly lower than Debye temperature of 1860 K for single crystal diamond. The quality factors of different resonators increased as the cantilevers were cooled from 300 K to 30 K and with the hydrogen termination of the cantilever surface. The results indicate that surface and bulk defects significantly contribute to the observed dissipation as well as the mechanical softening in UNCD resonators.

Evidence of universality in the dynamical response of micromechanical diamond resonators at millikelvin temperatures, Matthias Imboden, Pritiraj Mohanty, Boston University — We report Kelvin to millikelvin-temperature measurements of dissipation and frequency shift in megahertz-range resonators fabricated from ultrananocrystalline diamond. Frequency shift $\delta f/f_0$ and dissipation $Q^{-1}$ demonstrate temperature dependence in the millikelvin range similar to that predicted by the glass model of tunneling two level systems. The logarithmic temperature dependence $\delta f/f_0$ is in good agreement with such models, which include phonon relaxation and phonon resonant absorption. Dissipation shows a weak power law, $Q^{-1} \sim T^{1/3}$, followed by saturation at low temperature. A comparison of both the scaled frequency shift and dissipation in equivalent micromechanical structures made of single-crystal silicon and gallium arsenide indicates universality in the dynamical response.

Small to medium atomic size-mismatch leads to alloy phase-separation yet huge mismatch can lead to ordering, Xiwen Zhang, Giancarlo Trimarchi, Mayeul D’Avezac, Alex Zunger, National Renewable Energy Lab., Golden, CO 80401 — Most alkali halide alloys AX-BX (where A and B are alkali elements and X = F, Cl, Br, or I) are expected to have miscibility gaps (phase separation) which increases with the lattice mismatch. Even though LiO-RbX and LiX-CsX with lattice mismatches of 20 – 33% and 19 – 40% respectively might be expected to have pronounced miscibility gaps, they were experimentally found to have ordered structures. Here, we investigate the possible stabilization of ordered compounds with respect to random configurations. In the family of LiNaBr$_2$, LiKBr$_2$, LiRbBr$_2$, and LiCsBr$_2$, we find that as the lattice mismatch increases, the formation enthalpy of the random structure increases, (mainly due to the volume deformation), but the formation enthalpy of the ordered structure decreases becoming negative for the latter two. The ordered structures consist of distorted LiX$_4$ tetrahedral arranged in layers, with Rb (or Cs) sitting between layers at the center of the resulting triangular prism. We analyze the origin of ordering from the large local distortion induced by the huge lattice mismatch.

Funded by DOE-SC-BES-MSED through NREL Contract DE-AC36-08GO28308

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X11 DAMOP: Fermions in Optical Lattices II

Non-Equilibrium Enhancement of Superfluidity in a Trapped Fermi Gas, Andrew Robertson, Victor Galitski, University of Maryland, College Park — In 1970, Eliashberg showed that superconductivity could be stimulated by pushing the quasiparticle spectrum out of equilibrium and to higher energies using a periodic perturbation with a frequency of the order of the superconducting gap (Eliashberg, JETP Lett. 11, 114 (1970)). This effect has been observed in thin films (TM Klappen et al. JLTP 26, 3-4 (1977)). The theory of this gap enhancement can be mapped onto a cold Fermi gas. We present here the theoretical framework for describing the stimulation of the BCS order parameter in an interacting Fermi gas by means of a periodic perturbation.
2:42PM X11.00002 Realizing the Strongly Correlated \(d\)-Wave Mott-Insulator State in a Fermionic Cold-Atom Optical Lattice\(^1\). MICHAEL PETERSON, CHUANWEI ZHANG, SUMANTA TEWARI, SANKAR DAS SARMA, University of Maryland — We show that a new state of matter, the \(d\)-wave Mott-insulator state (\(d\)-Mott state) (introduced recently by [H. Yao, W. F. Tsai, and S. A. Kivelson, Phys. Rev. B 76, 161104 (2007)]), which is characterized by a nonzero expectation value of a local plaquette operator embedded in an insulating state, can be engineered using ultracold atomic fermions in two-dimensional double-well optical lattices. We characterize and analyze the parameter regime where the \(d\)-Mott state is stable. We predict the testable signatures of the state in the time-of-flight measurements.

\(^1\)Work supported by ARO-DARPA.

2:54PM X11.00003 Spectral function of spinless fermions on a one-dimensional lattice. RODRIGO PEREIRA, KITP, STEVEN WHITE, UC Irvine, IAN AFFLECK, University of British Columbia — We study the spectral function of spinless fermions for an integrable lattice model away from half-filling. The sharp features of the spectral function at arbitrary momentum are argued to be power law singularities analogous to the x-ray edge singularity. Besides the singularity at the energy of the single-particle excitation, we find that at low fillings the spectral function can exhibit a second divergence associated with the formation of a \(p\)-wave antibound state. The predictions from the effective field theory are compared with numerical results from the time-dependent density matrix renormalization group.

3:06PM X11.00004 Superfluidity at the BEC-BCS crossover in two-dimensional Fermi gases with population and mass imbalance\(^1\). GARETH CONDUIT, University of Cambridge, PETER CONLON, University of Oxford, BEN SIMONS, University of Cambridge — We explore the zero-temperature phase behavior of a two-dimensional two-component atomic Fermi gas with population and mass imbalance in the regime of the BEC-BCS crossover. Working in the mean-field approximation, we show that the normal and homogeneous balanced superfluid phases are separated by an inhomogeneous superfluid phase of Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) type. We obtain an analytical expression for the line of continuous transitions separating the normal and inhomogeneous FFLO phases. We further show that the transition from the FFLO phase to the homogeneous balanced superfluid is discontinuous leading to phase separation. If the species have different masses, the superfluid phase is favored when the lighter species is in excess. We explore the implications of these findings for the properties of the two-component Fermi gas in the atomic trap geometry. Finally, we compare and contrast our findings with the predicted phase behavior of the electron-hole bilayer system. [1] Phys. Rev. A 77, 053617 (2008)

\(^1\)The authors acknowledge the financial support of the EPSRC.

3:18PM X11.00005 ABSTRACT WITHDRAWN —
4:18PM X11.00010 General Hubbard Model for Fermions in an Optical Lattice, JASON KESTNER, LUMING DUAN, FOCUS center and MCTP, Department of Physics, University of Michigan — For two-component fermions in an optical lattice, an effective general Hubbard model (GHM) with tunable on-site attraction/repulsion and occupation-dependent hopping rates emerges from very general arguments [1]. This model is quite interesting, containing as special cases both the t-J and the XXZ models. However, the experimental range of applicability and the connection between the model parameters and the actual experimental parameters must be determined explicitly. To this end, we have used a stochastic variational approach with correlated Gaussian wavepackets to numerically find the eigenstates of two atoms interacting in a 3D few-well lattice. By matching the variational spectrum of the GHM to the variational spectrum obtained, the validity of the model and the relationship between experimental and model parameters is determined. [1] L.-M. Duan, Euro. Phys. Lett. 81, 20001 (2008).

4:30PM X11.00011 ABSTRACT WITHDRAWN

4:42PM X11.00012 ABSTRACT WITHDRAWN

4:54PM X11.00013 Probing Nagaoka ferromagnetism in optical superlattices, JAVIER VON STECHER, JILA and Department of Physics, University of Colorado, Boulder, Colorado, EUGÈNE DEMLER, MIKAHIL LUKIN, Physics Department, Harvard University, Cambridge-MA, 20138, ANA MARIA REY, JILA and Department of Physics, University of Colorado, Boulder, Colorado — In 1966, Nagaoka predicted that interaction-induced ferromagnetism occurs in lattices with specific geometry when there is one electron fewer than in the half-filled system. Here, we describe a controllable method for observing Nagaoka Ferromagnetism in isolated quasiparticles (four lattice sites arranged in a square) created using optical superlattices. We next discuss the weakly coupled quasiparticles and suggest several approaches for creating systems exhibiting itinerant ferromagnetism.

5:06PM X11.00014 Competition between spin imbalance and mass imbalance in the 1D asymmetric Hubbard model, WEN-LONG LU, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong, ZHI-GUO WANG, Department of Physics, Tongji University, SHI-JIAN GU, HAI-QING LIN, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — In this talk, I will discuss the spin imbalance in the 1D asymmetric Hubbard model in the negative U region by the Bosonization method. A ground-state phase diagram has been obtained. We find that, unlike the $N_\uparrow = N_\downarrow$ case, there is no other phase transition in the ground state (always Singlet Superconducting) before it enters into the phase separation region, and the pairing correlation function is found to oscillate in real space (FFLO state). The maximum mode is only determined by difference of Fermi momenta, and the correlation exponent is determined by both the mass difference and spin polarization. $^1$This work is supported by HK RGC Grant 402107

5:18PM X11.00015 Spin-coherent and -incoherent Luttinger liquids in trapped ultracold atomic Fermi gases, PAATA KAKASHVILI, C. J. BOLECH, Rice University — Recent success in manipulating ultracold atomic systems allows to probe different strongly correlated regimes in one dimension. Experimentally, 1D tubes are defined by turning on a 2D optical lattice. Regimes such as the spin-coherent Luttinger liquid and the spin-incoherent Luttinger liquid can be realized by tuning the inter-atomic interaction strength and trap parameters. Due to the trap potential the density decreases near the edges of the tubes and the spin-incoherent regime is inevitably realized. In general, the spin-coherent Luttinger liquid regime in the center of the tube crosses over to its spin-incoherent counterpart at the edges. We identify the noise correlations of density fluctuations as a robust observable (uniquely suited in the context of trapped atomic gases) to discriminate between these two regimes. Finally, we address the concrete prospects of realizing and probing these phenomena experimentally using optical lattices.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X12 DMP DCMP: Structure and Morphology of Oxide Surfaces and Thin Films 308

2:30PM X12.00001 Finding stable α-quartz (0001) surface structures via simulations, YUN-WEN CHEN, CHAO CAO, HAI-PING CHENG, Department of Physics and Quantum Theory Project, University of Florida — Reconstruction of α-quartz (0001) surfaces is studied using combined classical molecular dynamics and density functional theory. Five reconstruction patterns are identified, including three (2 × 1) patterns and two (1 × 1) patterns. The energetically most stable surface structure is found to be a (2 × 1) reconstruction pattern, and several patterns can co-exist in a large scale surface. A combination of structures can explain the experimentally observed (2 × 2) diffraction pattern. $^1$Acknowledgement: this work is supported by the NSF under Grant No. DMR/ITR-0218957 and DMR-0804407.

2:42PM X12.00002 Investigation of stability issues of TCO barrier layers for CIGS devices during damp heat and dry heat exposures, RAJALAKSHMI SUNDARAMOORTHY, INGRID REPINS, DAVID ALBIN, JOHN PERN, XIANKAN LI, TIM GESSERT, THOMAS GENNETT, National Centre for Photovoltaics, National Renewable Energy Laboratory — The reliability of In$_2$O$_3$/SnO$_2$ (ITO) and In$_2$O$_3$/ZnO (IZO) as barrier layers for CuInGaSe$_2$ (CIGS) solar cells has been investigated. NREL’s high-efficiency CIGS devices are prepared using a three-stage process for the CIGS layer, and insulating ZnO and ZnO:Al as the (bi-layer) transparent conducting oxide (TCO) buffer and conducting layers, respectively. These CIGS devices are processed to explore the effectiveness of barrier layers of ITO and IZO sputtered at room temperature and at various temperatures. Devices are exposed to damp heat at 85°C and 85% relative humidity (RH) and dry heat conditions (85°C/∼0% RH). Some cells are also tested under 1-sun illumination and open-circuit voltage bias. Optical, electrical, structural, and imaging analyses are used to characterize the samples periodically before and after the exposures. Surface depth profiling and relative concentration of the elements present are analyzed using XPS. Results of these stability studies will be discussed. This abstract is subject to experimental verification using XPS.

2:54PM X12.00003 Scanning Tunneling Microscopy Study of a Vicinal Anatase TiO$_2$ Surface, SHAO-CHUN LI, OLGA DULUB, ULRRIKE DIEBOLD, Department of Physics, Tulane University, DEPARTMENT OF PHYSICS, TULANE UNIVERSITY COLLABORATION — Titanium dioxide finds versatile applications in various technical fields including gas sensing, coatings, pigments, heterogeneous catalysis, photocatalytic degradation of pollutants, and solar cells. TiO$_2$ is found in three main crystallographic phases: rutile, anatase and brookite. Rutile is the thermodynamically most stable form and is considered a model system for basic research. However, anatase TiO$_2$ is often considered to be catalytically more active than rutile for reasons not yet completely understood. In this work, using scanning tunneling microscopy (STM) and low energy electron diffraction (LEED), the structure of the anatase TiO$_2$(5 5T) surface, $\sim$10° vicinal to the $\sim$ lowest energy $\sim$ (101) plane, has been studied. The surface was found to facet into a structure composed of ridges with a uniform width of 5 lattice units. Based on atomically-resolved STM and electron counting rules, it is proposed that the sides of the ridges are parallel to (1 10) and (1 12) planes. These sides might be reconstructed to stabilize the microfaceted structure. Vapor-deposited gold shows pronounced clustering between the ridges, indicating a one-dimensional template effect of the vicinal surface, which supports denser and more uniformly sized Au clusters, as compared to the flat (101) surface.
References:


4:30PM X12.00011 Tunable Metallicity at the Surface of La$_{5/8}$Ca$_{3/8}$MnO$_3$/SrTiO$_3$ Thin Films. KENJI FUCHIGAMI, Oak Ridge National Laboratory / The Univ. Tennessee, ZHENG GAI, Oak Ridge National Laboratory, THOMAS Z. WARD, Oak Ridge National Laboratory / The Univ. Tennessee, LIFENG YIN, PAUL SNIJDERS, Oak Ridge National Laboratory, WARD PLUMMER, The Univ. Tennessee, JIAN SHEN, Oak Ridge National Laboratory / The Univ. Tennessee — A series of in-situ STM studies of La$_{5/8}$Ca$_{3/8}$MnO$_3$(001) thin films reveals that the surface metallicity can be tuned by extrinsic oxygen doping at the surface. By in-situ annealing with or without oxygen, we can convert the surface back and forth between a ( Å2, x Å 2, Å45) reconstructed surface and a (1 x 1) surface. Electrical properties of the surfaces are investigated by scanning tunneling microscopy (STM). I–V curves clearly show that the oxygen doping renders the surface insulating while the (1 x 1) surface without the oxygen doping is metallic. Structural models and their correlation to the surface metallicity have been proposed.

4:42PM X12.00012 Surface properties of ultrathin ferroelectric films in external electric field. RENAT SABIRIANOV, University of Nebraska at Omaha, MINORU OTANI, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, OSAMU SUGINO, University of Tokyo — The electric polarization of free standing ultrathin films of BaTiO$_3$ is analyzed using pseudopotential plane wave calculations within effective screening medium method. The polarization loop in asymmetrically terminated (Pb,Ba)TiO$_3$ film is biased, providing the existence of polarization without applied electric voltage across the film. We attribute the origin of bias to a creation of a bias field due to difference in surface work functions of TiO$_2$ and BaO terminations. These results in the formation of surface polarizations at each termination and inhomogeneous polarization profile across the thickness of the film. We show that the surface develops in-plane component of polarization in paraelectric state, and also in case of the ferroelectric films when the electric field applied perpendicularly to the plane of the film.

4:54PM X12.00013 Growth and Characterization of EuTiO$_3$ films on SrTiO$_3$ (001). H. Q. WANG, School of Applied and Engineering Physics, and Cornell Center for Materials Research (CCMR), J. D. FERGUSON, Department of Materials Science and Engineering, and CCMR, A. R. WOLL, School of Applied and Engineering Physics, and Cornell High Energy Synchrontron Source. D. A. MULLER, School of Applied and Engineering Physics, and CCMR, J. D. BROCK, School of Applied and Engineering Physics, and CCMR, Cornell University, Ithaca, New York, USA — Ferroelectric films display a variety of interesting physical properties, and their heteroepitaxial structures are of significant interest in oxide electronics. EuTiO$_3$ and SrTiO$_3$ are nearly perfectly lattice matched and have the same valence structure, and are therefore well suited as a model system for the study of ferroelectric interfaces. One outstanding question about such interfaces concerns the factors that determine and limit atomic and electronic abruptness. In this work, several monolayer thick EuTiO$_3$ films are grown on single-crystal SrTiO$_3$ (001) substrates using Pulsed Laser Deposition (PLD). The growth mechanisms are probed by the combination of synchrotron based in situ small x-ray scattering (SAXS) and in situ reflection high energy electron diffraction (RHEED). The atomic-scale interfacial properties are investigated by high resolution Scanning Transmission Electron Microscopy (STEM) and spatially resolved Electron Energy Loss Spectroscopy (EELS).

5:06PM X12.00014 Density functional calculations of the structure of near-surface oxygen vacancies and electron localization on CeO$_2$(111). M. VERONICA GANDUGLIA-PIROVANO, Humboldt-University Berlin, Unter den Linden 6, 10099 Berlin, Germany, JUAREZ L.F. DA SILVA, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA, JOACHIM SAUER, Humboldt-University Berlin, Unter den Linden 6, 10099 Berlin, Germany — The use of ceria as a key component in catalysts and as an electrolyte for solid oxide fuel cells relies on its notable capability of storing and releasing oxygen. This property results from the facility of both formation and healing of oxygen vacancies in ceria. Several studies have been reported in the last years for reduced CeO$_2$(111), however, one of the most topical issues surrounding oxygen vacancies on CeO$_2$(111), namely, the relative stability of surface and subsurface defects, is still under intense debate. Using density functional theory with the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional as well as the DFT+U approach, we find subsurface vacancies with 3×2 periodicity to be energetically more favorable by 0.45 (HSE06), 0.47 (PBE+U), and 0.22 eV (LDA+U). The excess-electrons localize not on Ce ions which are nearest neighbor to the defect as priory suggested, but instead on those that are next-nearest neighbors. The excess-electron distribution and the preference for subsurface vacancies are explained in terms of defect-induced lattice relaxation effects.

5:18PM X12.00015 Interface structure determination of crystalline oxides on silicon using synchrotron x-ray diffraction. F.J. WALKER, J.W. REINER, A.M. KOLPK, Y. SEGAL, Yale University, Z. ZHANG, Argonne National Laboratory, D. SU, Y. ZHU, Brookhaven National Laboratory, M.S. SAWICKI, C.C. BROADBRIDGE, Southern Connecticut State University, S. ISMAIL-BEIJI, C.H. AHN, Yale University — As electronic devices are reduced in size, well controlled atomically abrupt interfaces become increasingly important. This is especially true for field effect devices where the conducting channel is only a few atoms thick. Here we discuss the experimental determination of the atomic structure of an interface for a model system, crystalline oxides on silicon, which contains the essential elements of field effect devices. For both BaO/Si and SrTiO$_3$/Si structures, we use a combination of synchrotron x-ray scattering, Z-contrast transmission electron microscopy and density functional theory to determine the structure. The combination of these approaches has led to a unique detailed model of the interface. We have discovered features of these interfaces that emerge during growth that can be used to understand important elements of the measured electrical properties and microscopically identify sources of fixed charge, interface traps and field-dependent mobility.


2:30PM X13.0001 System-averaged exchange-correlation holes and self interaction in second-row atoms. ANTONIO C. CANCEIO, Ball State University — Recent work is presented on the theoretical calculation of system-averaged exchange and correlation holes (intracules) for a pseudopotential model of the valence shell for the second row atoms Mg through Ar. Exchange holes are obtained from numerical Fourier transform methods and correlation holes from variational quantum Monte Carlo calculations using the method of correlated estimates. We observe scaling behavior in both exchange and correlation, following the known scaling of the valence density across the row, once self-interaction effects are taken into account. The holes are compared to density-functional models including LDA, GGA and related SIC approaches. We note a sizeable error due to self-interaction occurs in the same-spin channel of the correlation hole which persists for the LDA and GGA even after standard self-interaction corrections are applied. The effects of this error and proposed corrections to it on the total exchange-correlation energy will be discussed.
2:42PM X13.00002 Constraint-based, Single-point Approximate Kinetic Energy Functionals
FRANK E. HARRIS, Physics, University of Utah, V. V. KARASIEV, Instituto Venezolano de Investigaciones Cientificas, R. S. JONES, Loyola College of Maryland, S. B. TRICKEY, QTP, University of Florida — We work toward the development of orbital-free density functionals for the Kohn-Sham kinetic energy $T_K$ of a quality suitable for the computation of quantum-mechanical forces in multi-scale molecular dynamics simulations. The functionals are based on constraints applicable to the Pauli potential $v_p = 8T_D/n$, where $T_D = T_v + T_w$ and $T_v$ is the von Weizsäcker kinetic-energy functional. We review our progress to date, and exhibit functionals that do not generate spurious singularities and that produce chemical bonding in semi-quantitative agreement with Kohn-Sham computations and relevant experiments.

1Supported by U.S. NSF Grants PHY-0601758 and DMR-0325553

2:54PM X13.00003 Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets, WILLIAM GARBER, WEI KU, JAMES DAVENPORT, DMITRI VOLIA1, Brookhaven National Laboratory — A new development of first-principles electronic method will be presented based on direct energy functional minimization and bi-orthogonal wavelet basis set. The employment of bi-orthogonal basis allows systematically controlled accuracy while benefiting from the compact support that allows O(N) algorithms. Furthermore, utilization of the interpolating nature of the wavelet, together with the effectiveness of multi-resolution of wavelet, enables very efficient calculation without compromising accuracy. By avoiding solving eigenvalue equation as in standard Kohn-Sham framework, the method is easily extended to parallel algorithms, and allows simple implementation of various non-local functionals. In case of crystals, our method gives directly solution as Wannier functions, further utilizing their sparseness. This new development is ideal for easy implementation and accurate systematic benchmarking of various modern functionals, and holds the potential to attack very large systems such as nano-materials.

1currently postdoc at MIT

3:06PM X13.00004 Quenched Lieb-Oxford Satisfaction and Improved Performance for PBE-type Functionals
S. B. TRICKEY, QTP, Univ. Florida, V. MEDEL, A. VELA, Cinvestav, Mexico City — Success for the orbital-free DFT approach to Born-Oppenheimer forces for first-principles molecular dynamics requires progress on orbital-free exchange-correlation (XC) functionals to go along with newly developed orbital-free kinetic energy functionals [V.V. Karasiev et al. arXiv 0809.4798, J. Comput.-Aided Mat.Des. 13, 111 (2006)]. We report on development and testing of a non-empirical X functional which generalizes PBE X. It satisfies a reduced Lieb-Oxford bound by quenching to homogeneous electron gas behavior for large values of the inhomogeneity $s \propto |\nabla n|/n^{1/3}$ on the grounds that large $s$ often corresponds (counter-intuitively) to small, smooth density. Used with the PBE C functional, our X functional reduces mean absolute errors for small molecules by 20% or more with respect to conventional PBE XC. Used with LYP C (a semi-empirical combination), the performance also is improved relative to PBE-LYP.

3:18PM X13.00005 On the performance of Thomas-Fermi in periodic two-dimensional systems
LAZARO CALDERIN, MALCOLM J. STOTT, Department of Physics, Queen’s University, Kingston K7L 3N6, Ontario, Canada — The largest missing piece of a completely orbital free Density Functional Theory is the kinetic energy functional $T_K[n]$, and approximations for this are of interest. One of these expands $T_K$ in terms of density gradients with the Thomas-Fermi functional as the first term. But in three-dimensions the expansion appears not to converge, and the sixth and higher order corrections diverge for localized systems. In contrast, a number of authors have shown that the density gradient corrections all vanish in two-dimensions, while numerical test revealed that, even when not exact, TF is a very good approximation. That has been shown for the case of an impurity in a otherwise two-dimensional uniform electron gas. In this work we explore the validity of TF and linear response theory for a periodic two-dimensional system, a system that is likely to be more widely applicable.

1Acknowledgement: Work supported by NSERC of Canada.

3:30PM X13.00006 Effect of disorder on the electronic properties of strongly correlated systems within the dynamical cluster approximation
UNJONG YU, ABDOLMAJID NILI, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — We study the interplay of disorder and strong correlations on the electronic properties of highly correlated systems. We employ the dynamical cluster approximation (DCA) to include the effects of short-range correlations and alloy disorder beyond the coherent potential approximation (CPA). Our study focus on the double exchange model, relevant on the study of dilute magnetic semiconductors, and the periodic Anderson model to study heavy fermion compounds. We present results of several electronic properties as function of disorder strength, alloy concentration, and electron or hole doping.

1This work was supported by the National Science Foundation through OISE-0730290, DMR-0548011, and DMR-0706379.

3:42PM X13.00007 Basic Variables in Density Functional Theory in the Presence of a Magnetic Field
VIRAHT SAHNI, The Graduate Center CUNY, XIAOYIN PAN, Ningbo University — We have shown via a unitary or equivalently a gauge transformation that for a system of $N$ electrons in an external field $F = e\mathbf{A}/c$, the wave function $\Psi$ is in general a functional of the ground state density $\rho(\mathbf{r})$ and a gauge function $\alpha(\mathbf{R})$: $\mathbf{R} = \mathbf{r}_1, \ldots, \mathbf{r}_N$, i.e. $\Psi = \Psi[\rho, \alpha]$. The functions $\alpha(\mathbf{R})$ are arbitrary, the choice $\alpha(\mathbf{R}) = 0$ being equally valid. It is the presence of $\alpha(\mathbf{R})$ that ensures the wave function functional is gauge variant. Similarly, in the presence of a magnetic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, we show that in general the wave function is a functional of the density $\rho(\mathbf{r})$, the physical current density $\mathbf{j}(\mathbf{r})$, and a gauge function $\alpha(\mathbf{R})$: $\Psi = \Psi[\rho, \mathbf{j}(\mathbf{r}), \alpha]$. Again, the $\alpha(\mathbf{R})$ are arbitrary, the choice $\alpha(\mathbf{R}) = 0$ being valid. Hence, it is possible to construct a theory in which the basic variables are $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$. The generalized Hohenberg-Kohn theorems, as well as the equations for the noninteracting fermion Kohn-Sham system that reproduces the $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ of the interacting system of electrons, are derived.


2X.Pan: National Natural Science Foundation, China. Grant 10805029
3:45PM X13.00008 Projector Augmented Wave database with automatic parameter optimization

R.J. Snow, University of California Davis, A.F. Wright, Sandia National Laboratory, C.Y. Fong, University of California Davis — Projector Augmented Wave (PAW) parameter sets, similar to pseudopotential parameters, can be constructed in many ways. Due to a non-local expansion of projectors, the PAW method can include parameters for each angular momentum channel separately. While this gives the flexibility to optimize projectors individually, it also creates an unfathomable parameter space for searching for good parameter sets. To automatically search for good PAW sets, log derivative derivatives were analyzed numerically for matching with AE log-derivatives. Log-derivative matching, total energy convergence, and self-consistency errors found in density functionals. Since the Projector Augmented Wave (PAW) formalism ensures accurate evaluation of interaction integrals by controlling the multipole moments, it is a natural choice for implementing OEP within an efficient pseudopotential-like scheme. We developed a frozen core approximation scheme for the atomic all-electron OEP formalism, partitioning the exchange potential into core and valence contributions. The corresponding valence exchange pseudopotential for PAW, $V^\text{val} (r)$, can be derived in a similar way so that for $r > R_c$, $V^\text{val} (r) = V^\text{val} (r)$.

We have investigated the behavior of PAW-OEP basis, projector, and pseudopotential functions for several elements throughout the periodic table. Supported by NSF Grants DMR-0405456, 0427055, and 0705239.

1 Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

4:06PM X13.00009 A Projector Augmented Wave Formulation of the Optimized Effective Potential Formalism

Xiao Xu, N.A.W. Holzwarth, Wake Forest University — The optimized effective potential (OEP) or exact exchange (EXX) formalism has recently received renewed attention as a method which can improve the accuracy of density functional calculations by representing orbital-dependent potentials and avoiding self-interaction errors found in density functionals. Since the Projector Augmented Wave (PAW) formalism ensures accurate evaluation of interaction integrals by controlling the multipole moments, it is a natural choice for implementing OEP within an efficient pseudopotential-like scheme. We developed a frozen core approximation scheme for the atomic all-electron OEP formalism, partitioning the exchange potential into core and valence contributions. The corresponding valence exchange pseudopotential for PAW, $V^\text{val} (r)$, can be derived in a similar way so that for $r > R_c$, $V^\text{val} (r) = V^\text{val} (r)$.

We have investigated the behavior of PAW-OEP basis, projector, and pseudopotential functions for several elements throughout the periodic table.


4:18PM X13.00010 Density functional study of CO adsorption on d-metal surface using TPSS functional

Jianwei Sun, John Perdew, Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118 — Feibelman et al.[1] presented the puzzle of CO at the Pt(111) surface, showing that the LDA and Perdew-type GGA put the molecule at the wrong, high-coordination site. However, a recent study [2] showed that the BLYP yielded very satisfactory adsorption energies and the correct adsorption sites for CO adsorption at late 4d and 5d transition metal (111) surfaces, although at the price of large errors in the volume of the d metals. Since PBE and BLYP have similar accuracy, it seems the probable reason for the wrong adsorption site is due to the fact that the LDA and Perdew-type GGA’s are “jellium derived” and hence prefer a more delocalized bonding, rather than the fact that the LDA and GGA inaccurately describe the CO molecule’s chemical bond. TPSS meta-GGA is also “jellium derived”, but improves accuracy for molecules[4]. Therefore, as a possible candidate to identify the major reason for the wrong adsorption site, TPSS is used to calculate the adsorption energies and sites of CO on the d-metal surface in the more accurate geometric structure obtained by PBEsol[1]. [1] P.J. Feibelman et al, J. Phys. Chem. 105, 4018 (2001). [2] A. Stroppa and G. Kresse, New Journal of Physics 10, 063020 (2008). [3] V.N. Staroverov et al, J. Chem. Phys., 119, 12129 (2003). [4] J.P. Perdew et al, Phys. Rev. Lett., 100, 136406 (2008).

4:30PM X13.00011 Fully numerical all-electron solutions of the optimized effective potential equation for diatomic molecules

Adi Makmal, Weizmann Institute of Science, Israel, Stephan Kummel, University of Bayreuth, Germany, Leeor Kronik, Weizmann Institute of Science, Israel — We present an approach for fully numerical, all-electron solutions of the optimized effective potential equation within Kohn-Sham density functional theory for diatomic molecules. The approach is based on a real-space, prolate-spherical-coordinate grid for solving the all-electron Kohn-Sham equations and an iterative scheme for solving the optimized effective potential equation. The accuracy of this method is demonstrated by comparison with previously reported calculations and new benchmark fully numerical results for selected dimers are provided.

4:42PM X13.00012 Exchange Energy Density Functionals that reproduce the Linear Response Function of the Free Electron Gas

David García-Aldea, J.E. Alvelarlos, Dept. Física Fundamental, UNED — We present several nonlocal exchange energy density functionals that reproduce the linear response function of the free electron gas. These nonlocal functionals are constructed following a similar procedure used previously for nonlocal kinetic energy density functionals by Chacón-Alvarellos-Tarazona, García-González et al., Wang-Govind-Carter and García-Aldea-Alvelarlos. The exchange response function is not known but we have used the approximate response function developed by Utsumi and Ichimaru, even we must remark that the same ansatz can be used to reproduce any other response function with the same scaling properties. We have developed two families of new nonlocal functionals: one is constructed with a mathematical structure based on the LDA approximation — the Dirac functional for the exchange — and for the second one the structure of the second order gradient expansion approximation is took as a model. The functionals are constructed is such a way that they can be used in localized systems (using real space calculations) and in extended systems (using the momentum space, and achieving a quasilinear scaling with the system size if a constant reference electron density is defined).

4:54PM X13.00013 Non-local exchange-correlation term implemented into the density functional theory

Youky Ono, Center for Frontier Science, Chiba University, Koichi Kusakabe, Graduate School of Engineering Science, Osaka University, Takaishi Nakayama, Faculty of Science, Chiba University — The local density approximation (LDA) has serious limitation that this approximation cannot estimate the long-ranged (non-local) exchange-correlation interaction, as typified by the van der Waals (vdW) interaction. In this study we develop a method to calculate the vdW interaction based on the LDA together within the plasmon-pole approximation [1]. The computation code is developed as one of a module program of an existing first principle calculation package. Usefulness and efficiency of the method are confirmed by calculating the interaction energy of simple periodic systems. This method never relies on external parameters and/or on asymptotic model functions, and thus being applicable to any isolated 3 dimensional structures. [1] PRL 96, 073201 (2006), PRB 62, 6997 (2000), PRL 92, 246401 (2004).
When the average velocity verses mobility does not result in a Devil’s staircase, chaotic trajectories can be found.

In many instances, plotting the average velocity verses mobility results in a Devil’s staircase. When Devil’s staircases are seen, no chaotic behavior is present.

1. JAMES EAKINS, West Virginia University, JAMES VOPAL, West Liberty State College, BOYD EDWARDS, West Virginia University — Traveling-wave electrophoresis is a new method of separating charged analytes using a series of interlaced electrodes with time-varying electric potentials along a microchannel. This new representation allows for greatly reduced computation time and better description of the underlying mathematics is required in order to fully optimize this promising technology. As such, a new Fourier model of the electric potential inside the channel is introduced, along with preliminary computational results. This new representation allows for greatly reduced computation time and greater accuracy. Similarities and differences with other models are highlighted, as well as the dependence of the potential on the electrode and channel geometries. The movement of charged particles in response to the potential is examined, with several critical thresholds highlighted.

2. 2:30PM X14.00001 The dynamical origin of the zeta potential.

3. 2:42PM X14.00007 Trigonometric Model for Traveling Wave Electrophoresis.

Funding from NSF grants DMR-0647763 and EPS-0554328, and a WVU Research Corporation grant.
4:06PM X14.00009 Ac electroosmotic flows above coplanar electrodes. YONG KWEON SUH, Department of Mechanical Engineering, Dong-A University — Interactive numerical method has been proposed to calculate the ac electroosmotic flows above a pair of coplanar electrodes. The thin electrical triple layer (ETL) has been modeled by an asymptotic theory developed by the authors. The model corresponds to a simple dynamic equation for the surface charge density representing the integrated charge over the inner layer. Interactive calculation of the dynamic equation and the Laplace equation for several ac frequency then yielded steady-state distribution of potential and the potential drop across the Stern and inner layers. The Smoluchowski’s slip velocity was then determined from those two set of data and used as the boundary condition for the calculation of the Stokes’ flow above the electrodes. We have shown that our solutions compared well with the experimental data reported in the literature. We investigated the effect of various parameters on the slip velocity distribution, such as the ac frequency, the electrode length, the effective Stern-layer thickness and the adsorption coefficients.

4:18PM X14.00010 Detection and electrokinetic trapping of single fluorescent molecules in fused silica nanochannels. BRIAN CANFIELD, XIAOXUAN LI, WILLIAM HOFMEISTER, LLOYD M. DAVIS, University of Tennessee Space Institute — We describe experimental detection and electrokinetic trapping of single, fluorescently-labeled proteins confined within ~100 nm fluidic channels fabricated in fused silica. Though difficult to fabricate, the fused silica environment yields lower autofluorescence than borosilicate glass, which is especially advantageous given the low light level from single molecules. The molecules are dispersed in a buffer solution at ultralow concentration (~10^-12 M) to provide single-molecule occupancy of the sub-femtoliter probe volume within the nanochannel. Fluorescence is excited and collected in a custom-built confocal microscope, using two temporally interleaved beams from a modelocked dye laser focused to adjacent spots along the nanochannel. Detection is accomplished with custom single-photon avalanche diodes for time-resolved single-photon counting, and by using this time stamp information, a field-programmable gate array circuit board controls the electrokinetic trapping by modulating an applied voltage. Fluorescence correlation spectroscopy is also used to monitor the transport of molecules along the nanochannel. Electrokinetic transport can thus be characterized from changes in the autocorrelation function with voltage modulation.

4:30PM X14.00011 Microfluidic device for the electrokinetic manipulation of single molecules. JASON KING, LLOYD DAVIS, BRIAN CANFIELD, WILLIAM HOFMEISTER, University of Tennessee Space Institute, PHILIP SAMPSON, Vanderbilt University — We are developing a microfluidic device for three-dimensional electrokinetic manipulation of single fluorescent molecules in solution. The device consists of electrode pairs deposited onto glass cover slips by ion milling of a nickel template and sputtering of the electrode material. By use of a double Mach-Zehnder interferometer configuration, 40 fs Ti:Sapphire laser pulses (repetition rate 76 MHz) are split into four temporally interleaved pulses (effective rate 304 MHz), which are then focused to the vertices of a tetrahedron (approximately one micron per side) within the central electrode region to generate two-photon-excited fluorescence from single molecules. The time stamp data from this four-focus probe, collected with a custom fast-timing single-photon avalanche diode, enables characterization of particle motion through fluorescence cross-correlation spectroscopy.

4:42PM X14.00012 Microfluidic Channels under Magnetohydrodynamic (MHD) Convection. YOGENDRA M. PANTA, HYUN W. KIM, Youngstown State University, SHIZHI QIAN, Old Dominion University — Magnetohydrodynamic (MHD) effects have been widely known since many years. MHD effects are used to propel, stir, and pump fluids in various fluid applications especially in the field of microfluidics. Orthogonally aligned electric flux density and magnetic flux density were applied to straight and torroidal micro-channels both aligned perpendicular to the desired direction of fluid flow. Microfluidic MHD channels in straight and torroidal shapes were fabricated from a thin brass sheet sandwiched between two polycarbonate sheets patterned with two platinum electrodes in the channel walls from inside. When a potential difference of low magnitude (~ 1 mV) is applied across the electrodes, a current density J transmitted through the electrolyte solution results. In the presence of a magnetic field B, the orthogonal interaction between the resulting current density J and the magnetic field B induces Lorentz forces F (=J x B) which induce and drive fluid motion in the channel. This effect was applied to propel and pump the fluid in presence of a current carrying species both in a straight and torroidal micro-channels. Flow velocities were obtained linearly increasing with the magnetic flux densities. A drop of dye was placed into the solution to trace the path of moving fluid under MHD convection.

4:54PM X14.00013 Cell and Colloidal Substrates for Dielectrophoretic Microfluidic Immunoassays. JILL MAZUR, ZACHARY GAGNON, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering — Dielectrophoresis (DEP) is a term commonly used to describe the field induced polarization and translational motion of a polarizable particle in a non-uniform AC field. The frequency at which the induced particle dipole goes to zero, known as the crossover frequency (cof), is highly dependent on the surface conductance of the particle. We have previously shown that DNA hybridization on the surface of a 100 nm functionalized silica particle leads to detectable surface conduction changes which make it possible to detect DNA hybridization reactions by simply measuring changes in particle suspension cof. In this work we present a similar detection scheme using novel colloidal and cell substrates as dielectrophoretic immunoensors. Aminated cell or nanocolloid surfaces are subjected to a polymer coating glutaraldehyde treatment followed by antibody coupling reaction for immunoassay based detection. By varying the polymer coating thickness on the colloidal or cell surface we demonstrate the ability to tune, stabilize the cell and colloid cof, and minimized non-specific adsorption of proteins. As such, a library of cof labeled colloids and cells are created and used for multiple antigen analysis. By measuring the colloid and cell specific DEP cof prior to and after antibody-antigen interaction we demonstrated the ability to perform rapid label free protein detection within a microfluidic device.
5:06PM X14.00014 AC Electrokinesis Cell Separation on a Microfluidic Device, ZACHARY GAGNON, University of Notre Dame, Dept. Chemical and Biomolecular Engineering, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering — Rapid cell separation and collection is demonstrated through the integration of electrokinetic pumps, dielectrophoretic (DEP) traps and field driven valves into a well designed microfluidic channel loop. We present the ground-up design and analysis of this fully functional microfluidic device for the rapid separation and collection of live and dead yeast cells and malaria red blood cells (RBCs) at low concentrations. DEP cell sorting and concentration schemes are based on the exploitation of cell specific DEP crossover frequencies (cof’s). A rigorous DEP study of yeast and RBCs is presented and used to determine optimal conditions for cell separation. By utilizing a glutaraldehyde crosslinking cell fixation reaction that is sensitive to cell membrane protein concentration, we demonstrate the ability to further amplify these differences between healthy and unhealthy cells as well as stabilize their DEP cof’s. Pumping is achieved with a new type of electrokinetic flow, AC electrothermal electro-osmosis (ETEO) and is shown to scale inversely with the field induced debye length and drive fluid velocities in excess of 6 mm/sec. The well characterized electrokinetic phenomena are integrated into a microchannel loop with a specifically designed electrode field penetration length for low concentration cell separation and concentration.

5:18PM X14.00015 Anomalous analyte dispersion at microchannel-nanocapillary membrane interfaces, JARROD SCHIFFBAUER, Physics Dept, West Virginia University, KATHLEEN KELLY, Chemistry Dept., West Virginia University, WILL BOOTH, Physics Dept., West Virginia University, JOSH FERNANDEZ, Chemical Engineering, Dept., West Virginia University, AARON TIMPERMAN, Chemistry Dept., West Virginia University, BOYD EDWARDS, Physics Dept. West Virginia University — The dispersion of a plug-like distribution of negatively charged fluorescent dye molecules inside a microchannel is studied by numerical analysis of a time-series of epifluorescence microscope images. The concentration is accomplished using a nanocapillary membrane (NCM) —based concentration device. Dispersion of the analyte after concentration is complete, i.e. after the applied voltage is removed, is of considerable technical interest as a limiting factor in the functionality of lab-on-a-chip concentration devices. Subsequent band-broadening is inconsistent with Taylor dispersion and is shown here to be influenced by the presence of charge-separation between the concentrated analyte and background buffer ions.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X15 DFD: Liquid Crystals II 316

2:30PM X15.00001 The Taming of the Screw: Nonlinear Interactions in Smectic Liquid Crystals, ELISABETTA MATSUMOTO, GARETH ALEXANDER, RANDALL KAMIEN, University of Pennsylvania — From the twist grain boundary phase to the smectic phases of bent core liquid crystals, beautiful and intricate textures composed of screw dislocations appear time and again in a wide variety of smectic systems; yet, little is known about the interactions of screw dislocations. The linear smectic free energy is not sufficient to describe the energetics of single screw dislocations, and superposition cannot shed light on the interaction of many such defects. The full rotationally invariant nonlinear smectic free energy provides insight into systems of multiple screw dislocations. Such nonlinear interactions allow us to begin to understand the stability of the bulk phases observed in both smectic A liquid crystals and their chiral smectic C* counterparts.

2:42PM X15.00002 Coalescence Dynamics Analysis Of Islands In Smectic A Freely Suspended Films1, ZOOM NGUYEN, University of Colorado, Boulder, CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK — We explore the coalescence dynamics of circular islands in smectic A freely suspended liquid crystal films. The process typically has two distinct stages. First, when the islands make contact initially, the thinner island wraps around the thicker one. These dynamics are fast and determined by the line tensions of the islands and by the film’s viscosity. Then the region that used to be the thicker island expands and eventually covers the whole merged island. This process which is dependent on the permeation between layers in addition to the line tension and viscosity, is much slower. The shapes of the islands are extracted from high speed camera images and compared with model calculations.

5:06PM X15.00014 AC Electrokinesis Cell Separation on a Microfluidic Device, ZACHARY GAGNON, University of Notre Dame, Dept. Chemical and Biomolecular Engineering, HSUEH-CHIA CHANG, University of Notre Dame, Department of Chemical and Biomolecular Engineering — Rapid cell separation and collection is demonstrated through the integration of electrokinetic pumps, dielectrophoretic (DEP) traps and field driven valves into a well designed microfluidic channel loop. We present the ground-up design and analysis of this fully functional microfluidic device for the rapid separation and collection of live and dead yeast cells and malaria red blood cells (RBCs) at low concentrations. DEP cell sorting and concentration schemes are based on the exploitation of cell specific DEP crossover frequencies (cof’s). A rigorous DEP study of yeast and RBCs is presented and used to determine optimal conditions for cell separation. By utilizing a glutaraldehyde crosslinking cell fixation reaction that is sensitive to cell membrane protein concentration, we demonstrate the ability to further amplify these differences between healthy and unhealthy cells as well as stabilize their DEP cof’s. Pumping is achieved with a new type of electrokinetic flow, AC electrothermal electro-osmosis (ETEO) and is shown to scale inversely with the field induced debye length and drive fluid velocities in excess of 6 mm/sec. The well characterized electrokinetic phenomena are integrated into a microchannel loop with a specifically designed electrode field penetration length for low concentration cell separation and concentration.

2:30PM X15.00001 The Taming of the Screw: Nonlinear Interactions in Smectic Liquid Crystals, ELISABETTA MATSUMOTO, GARETH ALEXANDER, RANDALL KAMIEN, University of Pennsylvania — From the twist grain boundary phase to the smectic phases of bent core liquid crystals, beautiful and intricate textures composed of screw dislocations appear time and again in a wide variety of smectic systems; yet, little is known about the interactions of screw dislocations. The linear smectic free energy is not sufficient to describe the energetics of single screw dislocations, and superposition cannot shed light on the interaction of many such defects. The full rotationally invariant nonlinear smectic free energy provides insight into systems of multiple screw dislocations. Such nonlinear interactions allow us to begin to understand the stability of the bulk phases observed in both smectic A liquid crystals and their chiral smectic C* counterparts.

1 This work was supported by NASA Grant NAG-NNC04G508 and NSF MRSEC Grant No. DMR 0213918

2:54PM X15.00003 Orientational fluctuation study in nematic liquid crystals by high speed micrograph, BEOM-JIN YOON, MIN SANG PARK, School of Polymer, Textile, and Fiber Engineering, Georgia Institute of Technology, JUNG O. PARK, School of Polymer, Textile, and Fiber Engineering, Center for Advanced Research on Optical Microscopy, Georgia Institute of Technology, MOHAN SRINIVASARAO1, School of Polymer, Textile, and Fiber Engineering, School of Chemistry and Biochemistry, Center for Advanced Research on Optical Microscopy — The orientational fluctuations in uniaxial and biaxial nematic liquid crystals were investigated with a polarized microscope and a high speed TV camera. Liquid crystals usually have fluctuations with respect to their director, even when the molecular axes tend to be aligned to each other. These fluctuations are sufficiently slow and large, have long wave length and increase with temperature. Herein, we describe our study on fluctuation dynamics by direct observations in real space, while it has been typically done by the photon scattering in reciprocal space. The twinkling of liquid crystals due to orientational fluctuations were observed with a high speed camera up to 500 frames/sec. The time correlation function of the intensity was computed via 2D spatial Fourier transform of each image and then the relaxation frequency was estimated from it. The elastic constant to the viscosity ratio was computed from the relaxation frequency. This approach provides facile route to analyze fluctuation dynamics in liquid crystals.

1 All of Dr. Mohan Srinivasarao’s school and center is at Georgia Institute of Technology.
3:18PM X15.00005 Behavior of Focal Conic Defects in Shear Flow, SOURAV CHATTERJEE, SHELLEY ANNA, Carnegie Mellon University — The rheology of layered liquids is influenced to a large extent by defects present in the system, especially in small gaps. Toroidal focal conic defects are a common type of defect in small molecule layered liquids. We present a study of the influence of flow on focal conic defects in smectic liquid crystals, generated by antagonistic boundary condition at the surfaces. The defects are confined in gaps of the order of tens of microns and are subject to simple shear. The sizes of the focal conic defects vary with the gap size, and hence visual observations are made as to how the gap influences the dynamics of the focal conic defects in a shear flow. We also observe instabilities in initially defect free samples that lead to the creation of defects. The results offer insight into the complex relationship between defects and flow.

3:30PM X15.00006 Polarization current as evidence of local anticlinic correlations in de Vries smectics\(^1\), Z. V. SMITH, P. D. BEALE, R.-F. SHAO, L. WANG, D. M. WALBA, N. A. CLARK, M. A. GLASER, LCMRC, U. of Colorado, Boulder — Previous theoretical work on the electrooptic response of chiral de Vries SmA materials based on the electric field-induced reorientation of independent tilt domains [J. V. Selinger et al., Phys. Rev. E 64, 061705 (2001)] fails to account for the sigmoidal dependence of induced polarization (P) on field (E) seen in some materials. To account for this behavior, we model de Vries smectics as ensembles of small but finite anticlinic tilt domains. Within each domain, interlayer tilt coupling favors anticlinic interfaces, but the finite range of in-layer tilt correlations leads to thermally activated synclinic interfaces and a finite tilt correlation length along the layer normal. This model, equivalent to a generalized one-dimensional XY model in an external field with quadratic and quartic nearest-neighbor interactions, is studied by Monte Carlo simulation and transfer matrix methods. The model successfully reproduces the dependence of P on E for a specific material (W530), and yields physical parameters such as the in-layer correlation length and effective interlayer tilt coupling. The predicted anticlinic tilt correlations should be observable as diffuse superlattice reflections in polarized resonant x-ray scattering experiments.

\(^{1}\) Work supported by NSF MRSEC Grant DMR-0820579

4:20PM X15.00007 A one order parameter tensor description of biaxial nematic liquid crystals, XIAOYU ZHENG, Department of Mathematical Sciences, Kent State University, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — We present a simple one order parameter tensor mean field theory of biaxial nematic liquid crystals. We construct the free energy from molecular interactions, identify the components of the order parameter tensors, and obtain self-consistent equations, which are then solved numerically. The phase behavior is described via a 3D phase diagram. We discuss the connection between molecular properties and the coefficients in the Landau expansion.

4:40PM X15.00008 Elasticities and viscosities of a lyotropic chromonic nematic liquid crystal, KRISHNA NEUPANE, Kent State University, YURI NASTISHIN, Institute of Physical Optics, Lviv, Ukraine, ALAN BALDWIN, OLEG LAVRENTOVICH, SAMUEL SPRUNT, Kent State University — We have performed dynamic light scattering studies of the elastic moduli and viscosity coefficients in a uniformly aligned sample of a lyotropic chromonic nematic formed by 14 wt. % water solution of Disodium Cromoglycate \([1]\). These parameters show a significant anisotropy. In particular, the bend and splay moduli \(K_{11}\) and \(K_{13}\) are an order of magnitude higher than the twist modulus \(K_{22}\), and the ratio \(K_{13}/K_{11}\) shows an anomalous increase in temperature, which we attribute to the shortening of the aggregates. The bend viscosity is three orders of magnitude smaller than the splay and twist viscosities; all viscosity coefficients exhibit a strong temperature dependence.


4:06PM X15.00009 Reflection and transmission coefficients of a cholesteric liquid crystal film with a negative dielectric coefficient\(^1\), SABRINA RELAIX, WENYI CAO, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — A cholesteric liquid crystal (CLC) is a periodic dielectric structure where simple analytic solutions of Maxwell’s equations exist: light propagating along the helical axis has been first described by Mauguin in 1911 \([1]\), for wavelengths much smaller than the helical pitch, and was formulated more generally by de Vries in 1951 \([2]\). The analytical solutions are for bulk CLCs and do not describe the optical properties of a finite thickness CLC film. Recently, analytic expressions for the reflection and transmission coefficients of a CLC slab have been obtained by solving Maxwell’s equations and satisfying boundary conditions \([3,4]\), providing results for thick slabs which go beyond the limitation of numerical methods. We discuss how these results are modified when one of the dielectric coefficients is negative. We explore the connection with hyperbolic dispersion and negative index materials. \([1]\) C. Mauguin, Bull. Soc. Fr. Miner. Cristallogr. 34, 6 (1911) \([2]\) H. de Vries, Acta Crystallogr. 4, 219 (1951) \([3]\) W. Cao, Ph.D. dissertation, Chemical Physics, Kent State University (2005) (http://e-L.org) \([4]\) S. Relaix, W. Cao and P. Palffy-Muhoray, to be published

\(^{1}\) This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

4:18PM X15.00010 Maier-Saupe Theory of Nematics in 4D, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University, XIAOYU ZHENG, Department of Mathematical Sciences, Kent State University — We extend the Maier-Saupe theory of nematics to 4 dimensions. We consider the interaction of cylindrically symmetric particles, and derive an effective single particle potential. Using this, we obtain the free energy and the self-consistent equation for the order parameter – a second rank traceless tensor. In 4D, the order parameter has three independent eigenvalues. We solve the self-consistent equation, and study the solutions as function of temperature. Our results give insight into the relation between orientational order parameters in different dimensions.

4:30PM X15.00011 Statistical mechanics of the flexoelectric effect in nematic liquid crystals\(^1\), SUBHAS DHAKAL, JONATHAN V. SELINGER, Kent State University — Flexoelectricity is the phenomenon in which polarization is induced by imposed deformations of the director field in nematic liquid crystals. Recent experiments \([1,2]\) have found that the flexoelectric effect is three orders of magnitude greater for bent-core liquid crystals than for conventional rod-like liquid crystals. To understand this experimental result, we develop a lattice model for the statistical mechanics of the flexoelectric effect. We perform Monte Carlo simulations and mean-field calculations to find the behavior as a function of interaction parameters, temperature, and applied electric field. The resulting phase diagram has four phases: isotropic, uniaxial nematic, biaxial nematic, and polar. In the uniaxial and biaxial nematic phases, there is a large splay or bend flexoelectric effect, which diverges as the system approaches the nematic-polar transition. This model may explain the large bend flexoelectric coefficient observed in bent-core liquid crystals, which have a tendency toward polar order. \([1]\) J. Harden, B. Mbanga, N. Eber, K. Fodor-Csorba, S. Sprunt, J. T. Glesson, and A. Jakli, Phys. Rev. Lett. 97, 157802 (2006). \([2]\) J. Harden, R. Teeling, J. T. Glesson, S. Sprunt, and A. Jakli, Phys. Rev. E 78, 031702 (2008).

\(^{1}\) This work was supported by NSF Grant DMR-0605889.
4:42PM X15.00012 Aggregates in Chromonic Liquid Crystal Phases of Aqueous Solutions of Sunset Yellow*, LEELA JOSHI, SHIN-WOONG KANG, DENA MAE AGRA-KOULMAN, SATYENDRA KUMAR, Department of Physics, Kent State University — Molecules of dye Sunset Yellow consist of flat poly-aromatic core and hydrophilic groups at the periphery. In aqueous environments, they self-organize into columnar aggregates mainly via $\pi - \pi$ interactions between aromatic cores. At high concentrations, dye aggregates develop orientational and positional orders to form the nematic (N) and columnar (C) mesophases. Synchrotron x-ray scattering and optical polarizing microscopy were used to better understand the growth of aggregates and mesophase formation. Average column height and their spatial organization strongly depend on concentration, temperature, and pH value of the solution. The aggregate size decreases with temperature exhibiting an Arrhenius behavior with mesophase dependent activation energy. A dramatic decrease in the aggregate size upon addition of HCI highlights their sensitivity to electrostatic interactions. *Work supported by grant NSF/DMR-086991.

4:54PM X15.00013 Aggregation Properties of the Chromonic Liquid Crystal Benzopurpurin 4B, CHRISTOPHER MCKITTERICK, PETER COLLINGS, Swarthmore College — Benzopurpurin 4B (BPP) is a textile dye very similar to the common indicator Congo Red. As is true for all chromonics, the absorption spectrum is concentration dependent at low concentrations. To estimate a free energy change for aggregation, it is higher than has been determined for other systems. Unlike other recently investigated chromonic liquid crystals, BPP forms a liquid crystal phase at extremely low concentrations, about 0.5 wt%. Also unlike these other chromonic liquid crystals, the aggregation kinetics are exceedingly slow. X-ray diffraction and light scattering measurements indicate that the aggregates of BPP are much larger than for chromonic systems that form liquid crystals at higher concentrations. BPP aggregates can be imaged using confocal microscopy, revealing a layer distribution centered at 3 $\mu$m for a solution forced through a 0.2 $\mu$m filter. Over days, the aggregates lengthen to well over 10 $\mu$m. The diameter of the aggregate images is slightly greater than the diffusion limit of the microscope, placing an upper limit on the diameter of 0.14 $\mu$m. These dimensions are consistent with the light scattering results.

5:06PM X15.00014 Generalized Nemato-hydrodynamic Boundary Conditions with Application to Bistable Twisted Nematic Liquid Crystal Displays1, ANGBO FANG, Department of Physics, Hong Kong University of Science and Technology, TIEZHENQ QIAN, Department of Mathematics, Hong Kong University of Science and Technology, PING SHENG, Department of Physics and the Institute of Nano Science and Technology, Hong Kong University of Science and Technology — Parallel to the highly successful Ericksen-Leslie hydrodynamic theory for the bulk behavior of nematic liquid crystals (NLC), we derive a set of coupled hydrodynamic boundary conditions to describe the NLC dynamics near NLC-solid interfaces. In our boundary conditions, translational flux (flow slippage) and rotational flux (surface director relaxation) are coupled according to the Onsager variational principle of least energy dissipation. The application of our boundary conditions to the truly bistable $\pi$-twist NLC cell reveals that the thus far overlooked translation-rotation dissipative coupling at solid surfaces can accelerate surface director relaxation and enhance the flow rate. This can be utilized to improve the performance of electro-optical nematic devices by lowering the required switching voltages and reducing the switching times.

1 A. Fang acknowledges support from the KAUST Global Research Partnership.

5:18PM X15.00015 Soft Micro- to Nanolithography Using Highly Periodic Smectic Liquid Crystal Defects, HEE-TAE JUNG, YUN HO KIM, Korea Advanced Institute of Science and Technology, DONG-KI YOON, Samsung Electronics, HYEON SU JEONG, Korea Advanced Institute of Science and Technology, ORGANIC OPTO-ELECTRONIC MATERIALS LAB, TEAM — Achieving perfect long-range order with soft building blocks at high speed and high resolution is one of the most exciting interdisciplinary research areas in current materials science and nano-biotechnology. Here, we have developed highly periodic patterns with sub-micrometer features over large-areas using toric focal conic domains (TFCDs) originating from smectic liquid crystal (LC). TFCDs are accomplished by precisely controlling the surface and interfacial properties of smectic LC. In order to apply the smectic liquid crystal defect arrays in lithography, the hexagonal arrays of domain patterns are used as molds for ultraviolet (UV) curable polymers, thereby providing LC defect stamps with high spatial resolution over large areas. Our method was further utilized to transfer patterns with sub-micrometer features from the polymer stamp surface to a secondary surface by microcontact printing ($\mu$-CP). The patterning method based on LC defects has significant advantages over existing lithographic approaches: 1) the masters and stamps are easy to fabricate, 2) the masters and stamps provide long-range surface ordering over large-areas, 3) the periodic arrays are formed quickly in several seconds, and 4) the stamps can generate feature sizes on the micrometer and submicrometer length scales, and 5) the methodology offers the possibility of controlling the array geometry by altering the geometry of the confining channels.

Thursday, March 19, 2009 2:30PM - 4:42PM
Session X16 DCMP: Liquid Helium 317

2:30PM X16.00001 Measurements of the Thermal Conductivity of Vycor Glass filled with Superfluid $^4$He1, WILLIAM TIERNAN, Mesa State College, Grand Junction, CO and Univ. of Mass. Amherst, MA, SILVIA IONSECU, MICHAEL RAY, ROBERT HALLOCK, Univ. of Mass. Amherst, MA — We report on experiments designed to measure the thermal conductivity of Vycor filled with superfluid $^4$He for temperatures in the range 1.2 - 2.0 K and pressures from 2 - 30 atm. The experimental apparatus, which consists of a rod of Vycor held in a stainless steel tube, will be described. We will report available results for the thermal conductivity as a function of temperature and pressure.

1 Supported by the NSF

2:42PM X16.00002 Phonon-roton modes, superfluidity and a Bose glass phase in nanoscale liquid $^4$He, JACQUES BOSSY, Institut Neel, CNRS-UJF, Grenoble, JONATHAN PEARCE, National Physical Laboratory, HELMUT SCHOBER, Institut Laue Langevin, Grenoble, HENRY GLYDE, university of Delaware — We present neutron scattering measurements of the elementary phonon-roton modes of liquid $^4$He confined in nanoporous media. The aim is to compare phonon-roton (P-R) and superfluid density measurements in helium at nanoscales and in disorder. A specific goal is to determine the relation between temperature and pressure in which well defined phonon-roton modes (and therefore BEC) exist and compare this with the superfluid phase region, i.e. with the superfluid-normal phase critical temperature $T_c$ and pressure $p_c$ in porous media. We find well defined P-R modes (BEC) extend to temperatures above $T_c$ (up to $T_s = 2.17$ K at SVP) and to pressures above $p_c$ (up to a pressure $p = 36.3-36.8$ bars at $T = 0$ but no modes above this pressure [1]). This suggests that there is a Bose glass phase consisting of local regions of BEC separated by normal liquid so that there is no phase coherence across the sample lying between the superfluid and normal liquid phase. The Bose glass phase spans the superfluid phase at all $p$ and $T$. We compare this phase diagram with other dirty Bose systems. [1] Bossy et al. Phys. Rev. Lett. 101, 025301 (2008), Phys. Rev. B (in press)(2008)
2:54PM X16.00003 Thin $^4$He films on Nano-porous Diblock Copolymer Substrates. John Cummins, Amherst, MA, Robert Hallock, Amherst, MA — In recent years diblock copolymer templates have been a focus of attention due to their potential uses in nano-scale systems. The ability to produce regular arrays of cylindrical pores has applications in areas such as the production of nanowires and magnetic storage. Porous polymer films made by diblock copolymer techniques provide an interesting substrate for helium. Previously studied porous geometries e.g. nucleopore, anopore, aerogel, vycor, and porous aluminia have provided interesting insights into capillary condensation, the Kosterlitz-Thouless transition and hysteresis. Here we report on the study of thin superfluid $^4$He films on diblock copolymer substrates by means of quartz crystal microbalance techniques.

3:06PM X16.00004 Evidence of a Proximity Effect in Liquid Helium. Mark O. Kimball, Justin K. Perron, Francis M. Gasparini, University at Buffalo, The State University of New York — We report measurements of the specific heat of helium confined to boxes connected via a 32 nm thick film. The spacing between the boxes is approximately 4 μm edge-to-edge. The specific heat is compared to a similar measurement of helium confined to the same size boxes where the spacing between boxes is 2 μm. Evidence of a coupling between the boxes in the tighter packed array is seen in a temperature region where the filling film is in the normal state. We also report measurements of the superfluid fraction of the film connecting the boxes in the present experiment. The superfluid state persists to higher temperatures than that expected on the basis of finite-size scaling for a 32 nm film. At the temperatures where the measurement of the film occurs, the helium in the boxes is already superfluid indicating, perhaps, the modification in behavior of a thin film in proximity to larger regions of superfluid.

3:18PM X16.00005 A Novel Method to Create Multielectron Bubbles. Jeiping Fang, Anatoly Dementyev, Harvard University, Jacques Tempere, Universiteit Antwerpen, Isac Silbera, Harvard University — A multielectron bubble (MEB) in liquid helium is a fascinating object with a spherical two-dimensional electron gas on its surface. Recent theoretical studies of MEBs discuss a plethora of new phenomena. We describe a novel way of creating MEBs and discuss possible ways of trapping them. An electrically heated tungsten filament submerged in superfluid helium is surrounded by a vapor sheath containing electrons due to thermionic emission. We were able to pull MEBs from the sheath by applying electric fields up to 15 kV/cm. The motion of MEBs was captured using a high-speed camera (6400 frames/sec). The trajectory of bubbles was clearly influenced by the electric field, which proved that bubbles were charged. In a separate experiment we measured the charge of such an MEB to be as high as 10$^{-5}$ C. We plan to trap MEBs using electromagnetic trap, which will enable extensive experimental studies of these elusive but exciting objects.

3:30PM X16.00006 Phase diagram for helium films on lithium substrates. E. Van Cleve, J. C. Burton, P. Tabor, University of California, Irvine — We have used an in situ cryogenic pulsed laser deposition system to deposit a lithium film onto a quartz crystal microbalance. Helium 4 adsorption isotherms were measured on a lithium substrate between 2K and 0.6K. Features of these isotherms such as superfluid mass decoupling and variations in the dissipation were used to construct a phase diagram for helium films including the KT line and the 2D liquid-vapor coexistence region. The liquid-vapor critical temperature is approximately 0.8K. The KT transition is anomalous inside the 2D liquid-vapor coexistence region, occurring at constant sub-monolayer coverage independent of temperature. No inert solid-like layers of helium form on lithium substrates, so superfluid films are in direct contact with the substrate. These results will be compared and contrasted with the behavior of helium on other intermediate strength substrates such as exfoliated graphite pre-plated with hydrogen, sodium and magnesium.

3:42PM X16.00007 Quantized vortices and superflow in arbitrary dimensions: Structure, energetics and dynamics. Florin Bora, Paul Goldbart, University of Illinois at Urbana-Champaign — The structure and energetics of superflow around quantized vortices, and the motion inherited by these vortices from this superflow, are explored for the superfluidity of helium-four in arbitrary dimensions. The vortices may be idealized as objects of co-dimension two, such as two-dimensional surfaces in the case of four-dimensional superfluidity. The energy of the superflow is found to take on a simple form for vortices that are smooth and asymptotically large, compared with the vortex core size. The motion of vortices is analyzed in general, as well as for the special cases of hyper-spherical and weakly distorted hyper-planar vortices. In all dimensions, vortex motion reflects vortex geometry. In dimension four and higher, this includes not only extrinsic but also intrinsic aspects of the vortex shape. For the generalizations of the vortex rings of three dimensional superfluidity, the energy-momentum relation is determined. Simple scaling arguments recover the essential features of these results, up to numerical and logarithmic factors.

3:54PM X16.00008 $^3$He Spin Pump. A. Yamaguchi, H. Ishimoto, Institute for Solid State Physics, University of Tokyo, H. Kojima, Rutgers University — The superfluid component of $^3$He A$_1$ phase is spin-polarized. The process of forcing the superfluid component through a spin filtering structure, in a manner of mechano-magnetic effect, can be used to increase the spin polarization beyond the equilibrium under a given applied magnetic field. We have constructed a test cell in which a glass capillary array acts as the spin (and entropy) filter and an electrostatically actuated diaphragm forces the superfluid flow through it. Preliminary results show that a maximum relative increase of polarization by 50% could be achieved. The maximum increase in polarization appears to be limited by the critical superfluid flow through the channels in the glass capillary array. The dependence of the observed effects on temperature, pressure and magnetic field will be presented.

4:06PM X16.00009 The Spin Diffusion Coefficient of Superfluid $^3$He in the A$_1$- phase. Ayodeji AwoBode, Anthony Leggett, University of Illinois at Urbana Champaign — Using the Boltzmann kinetic approach and perturbation theory, an approximate expression describing the variation with temperature of the spin diffusion coefficient in the A$_1$-phase of $^3$He is derived. It is observed that for temperatures close to the transition temperature $T_c$, the spin diffusion coefficient $D \sim (T_c - T)^{1/2} + \text{const}$. Comparison of the theoretical result with related experimental measurements is discussed.
in superconductors. For the B-like superfluid phase of\textsuperscript{3}He in 98\% porosity aerogel for several different pressures in zero magnetic field \cite{1}. It revealed and confirmed many interesting features directly associated with impurity scattering: collisional drag effect, absence of zero sound crossover and order parameter collective modes, and gapless superfluidity. In this work, we report an experimental effort to uncover the detailed gap structure that is expected to be significantly modified by the presence of impurity scattering. We conducted frequency dependent attenuation measurements, which might shed light on this problem as a tunneling experiment does in superconductors. For the B-like superfluid phase of\textsuperscript{3}He in 98\% aerogel, we report sound attenuation measurements performed between 14 and 33 bar, while using four frequencies between 3.7 and 11.2 MHz.


\textsuperscript{3}This work is supported by NSF through DMR-0239483 and 0803516 (YL), DMR-0701400 (MWM), DMR-0654118 (NHMFL), and the State of Florida.

4:30PM X16.00011 Superfluid \textsuperscript{3}He in Anisotropic Aerogels\textsuperscript{1}. JOHANNES POLLANEN, JOHN P. DAVIS, BENJAMIN REDDY, KENT R. SHIRER, HYOUNGSOON CHOI, WILLIAM J. GANNON, CHARLES A. COLLET, WILLIAM P. HALPERIN, Northwestern University — Anisotropic quasiparticle scattering has been predicted to modify the properties of superfluid\textsuperscript{3}He in high porosity silica aerogels\textsuperscript{2}. For example, anisotropic scattering produced by axial compression (or elongation) of the aerogel has been predicted to stabilize the axial (or polar) state of superfluid\textsuperscript{3}He. We have used a transverse acoustic interference method to determine the phase diagram of superfluid\textsuperscript{3}He in a 98\% porous silica aerogel subjected to 17\% axial compression. We have found that this uniform axial anisotropy does not increase the stable region of A-like phase but does inhibit the nucleation of the B-phase at low pressure. We have performed optical cross-polarization experiments\textsuperscript{3} to verify the presence and uniformity of the anisotropy in the aerogel samples. Additionally, we are performing nuclear magnetic resonance experiments on superfluid\textsuperscript{3}He in aerogels with anisotropy introduced with either axial or radial compression.

\textsuperscript{1}This work was supported by the National Science Foundation, DMR-0703656.


Thursday, March 19, 2009 2:30PM - 5:18PM –
Session X17 GQI: Semiconducting Qubits II 318

2:30PM X17.00001 Effect of Substrate Doping in Relaxed SiGe Buffers on Strained Si 2DEG Quantum Devices. KUN YAO, MIKHAIL GAEVSKI, Princeton University, ALEXANDER CHERNYSHOV, LEONID ROKHINSON, Purdue University, CURTIN MIKE, JI.SOO PARK, JAMES FIORENZA, ANTHONY LOCHTEFELD, AmberWave Systems, JAMES STURM, Princeton University — We describe the impact of Si substrate doping on the substrate leakage in strained Si two-dimensional electron gases (2DEG) on SiGe relaxed graded buffers and on quantum devices fabricated from the 2DEG. The best commercially available high quality SiGe relaxed buffers with 30\% Ge content, grown at temperature above 1000\°C, have very low threading dislocation density (<1E5cm\textsuperscript{-2}). Subsequent strained Si/SiGe heterostructures were grown at 625-700\°C in a rapid thermal chemical vapor deposition (RTCVD). However, it is shown that the substrate doping (Arsenic) contributes to leakage current origin in relaxed buffers at liquid helium temperatures if the starting Si substrate is heavily doped (~5E17cm\textsuperscript{-2}). The leakage can be attributed to enhanced dopant diffusion along misfit dislocations and high diffusion rate of As in SiGe. The leakage current makes side gating of nanostructures in the 2DEG impossible. With a lightly doped substrate, to avoid leakage the structure has a high quality 2DEG and successful side gating of a 2DEG quantum dot for a quantum point contact. This work is supported by the NSA under ARO contract number W911NF-05-1-0437.

2:42PM X17.00002 Robust Fabrication Techniques for Si/SiGe Quantum Dots. MINGYUN YUAN, FENG PAN, TIM GILHEART, JOEL STETTENHEIM, MUSTAFA BAL, Dartmouth College, D. E. SAVAGE, M. A. ERIKSSON, University of Wisconsin-Madison, A. J. RIMBERG, Dartmouth College — Si/SiGe quantum dots promise a long spin coherence time due to reduced electron-nuclear spin interaction. Nevertheless, successful device yield has been limited in this novel material system due to difficulties in producing reliable ohmic contacts and Schottky gates. We have successfully developed fabrication processes that produce robust ohmic contacts and non-leaky Schottky gates. The ohmic contacts typically have a two-probe resistance of a few tens of kilohms and the Schottky gates have no detectable leakage current up to an applied voltage of -5 V. In typical devices we are able to pinch off the quantum point contacts with a voltage range between -1.5 V to -4.5 V. Recent experimental results will be discussed. This work was supported by the NSF under Grant No. DMR-0804483 and 0803516 (YL), DMR-0701400 (MWM), DMR-0654118 (NHMFL), and the State of Florida.

2:54PM X17.00003 Effect of Intervalley Mixing on Qubit Operation in SiGe Quantum Dot Structures\textsuperscript{1}. A. A. KISELEV, R. S. ROSS, B. H. FONG, M. F. GYURE, HRL Laboratories, Malibu, CA 90265 — We analyze the effects of valley degeneracy and intervalley mixing on single- and multi-electron states in (001) SiGe heterostructures, including effect of interface steps and variations in interface quality. We focus on the structure of two-electron states in both single and double quantum dot structures in the presence of valley degeneracy in the host material and the oscillatory behavior of exchange coupling in the presence of nonplanar heterointerfaces. We present modeling and simulation results relevant to the design of SiGe based accumulation-mode quantum-dot structures, especially CI calculation in presence of the intervalley mixing.

\textsuperscript{1}Sponsored by United States Department of Defense. Approved for Public Release, Distribution Unlimited.

3:06PM X17.00004 Transport and charge sensing in Si/SiGe double-quantum dots. CHRISTIE SIMMONS, MADHU THALAKULAM, E. K. SACKMANN, B. J. VAN BAEL, D. E. SAVAGE, M. G. LAGALLY, R. JOYNT, M. FRIESEN, S. N. COPPERSMITH, M. A. ERIKSSON, University of Wisconsin - Madison — Gated quantum dots in Si/SiGe are of interest because spins in silicon are weakly coupled to the host material. We demonstrate that Coulomb blockade measurements through a single quantum dot are well correlated with charge sensing in a nearby quantum point contact. Charge sensing enables the determination of the absolute number of electrons in the system, and we present data demonstrating a one-electron single quantum dot. Incorporated with a double quantum dot, charge sensing can be used to probe the inter-dot motion of a single electron at fixed total charge in the double dot. The tunnel coupling between the two dots directly effects the charge localization and thus the sharpness of this inter-dot transition. Here we demonstrate gated electrical control of the exchange coupling and thus an important step towards qubit implementation – showing a smooth transition between two well-isolated dots, two dots so strongly coupled that they act as a single large quantum dot, and the intermediate regime.

3:18PM X17.00005 Quantum dot crossbar circuits. CHRISTINE R. NOGUERA, University of Wisconsin – Madison — Quantum dot crossbars are a scalable method for performing quantum logic gates using multiple qubits. Quantum dot crossbars can be made with thin silicon films using electron-beam lithography and selective-area growth. The quantum dots are spaced at a distance that limits parasitic interactions with the gates. To show that a quantum dot crossbar can be made with current technology, we present experiments on arrays of quantum dots fabricated in a patterned silicon film using an electron-beam writer. We also present a crossbar design that is scalable to large numbers of qubits.
3:18PM X17.00005 Transient and stationary leakage current through a double quantum dot in the Pauli spin blockade regime, FARZAD QASSEMI MALOOMEH, WILLIAM A. COISH, FRANK K. WILHELM, Institute for Quantum Computing and Physics Department, University of Waterloo — We have calculated stationary and transient leakage current through a double quantum dot in the Pauli spin blockade regime. Quite remarkably, even in systems with inhomogeneous hyperfine coupling, we find that the leakage current is often controlled by spin-flip cotunneling processes with the leads. Our calculations show that these processes can be suppressed for one of the spin-triplet states by applying a small magnetic field, allowing for the preparation of a pure spin triplet. We have also found the transient effective charge passing through the double dot between blocking events, which can be strongly modified due to the spin-flip cotunneling processes. These results may explain features observed in several experiments.

3:30PM X17.00006 ABSTRACT WITHDRAWN

3:42PM X17.00007 Energy Dependent Tunneling in a Silicon Double Quantum Dot, MARK FRIESEN, University of Wisconsin-Madison, C. B. SIMMONS, NAKUL SHAJI, R. H. BLICK, S. N. COPPERSMITH, M. A. ERIKSSON — We study transport currents in a few-electron Si/Ge double quantum dot. A detailed analysis is made of the recently discovered phenomenon of lifetime enhanced transport (LET), in which current may flow in a regime typically considered to be blocked. To understand this effect, a rate equation model is developed, including both singlet and triplet transport channels. Making use of a simple model of tunneling across a quantum barrier, we map out the energy dependence of the tunneling. This allows us to obtain quantitative estimates for the tunneling rates and transport currents throughout the reverse bias regime. We are then able to identify both resonant and non-resonant phenomena, and provide a physical understanding of the different blockade regimes. In particular, we provide detailed predictions for the conditions under which LET may be observed.

3:54PM X17.00008 Charge transport in silicon double quantum dots, TED THORBECK, JQI, NIST and U. of Maryland, NEIL ZIMMERMAN, NIST, AKIRA FUJIWARA, YUKINORI ONO, YASUO TAKAHASHI, HIROSHI INOKAWA, NTT Basic Research Laboratory — Double quantum dots are an essential component for many schemes of semiconductor quantum computation. We will present results for transport through a silicon double quantum dot system. Our devices are formed by mesa-etching an SOI wafer to form a nanowire, and then poly-silicon gates are deposited. A global gate is used to invert and local gates form tunnel barriers isolating quantum dots and controlling the potential of the dots. Because the coupling between the two dots is controllable, a transition from a single dot, to two coupled dots, to two uncoupled dots is observed. We will analyze the resulting honeycomb diagram. We also hope to present results in the few electron regime.

4:06PM X17.00009 Modeling of Accumulation-Mode Quantum Dot Structures for Quantum Information Processing1, R. S. ROSS, A.A. KISELEV, B.H. FONG, M.F. GYURE, HRL Laboratories, Malibu, CA 90265 — We present modeling and simulation results relevant to the design of SiGe and III-V based accumulation-mode quantum-dot structures for use as electron-spin-based qubits. We have developed a self-consistent real-space multi-electron simulation tool to efficiently explore and optimize these structures. Specific practical issues we address include the design of double-quantum-well heterostructures, enhancement-gate-electrode design and quantum-dot electronic structure with attention to the effects of electrostatic gate action. We examine the addition and excited-state spectra of single quantum dots (QDs), the exchange coupling of nearest-neighbor quantum dots and the vertical tunneling behavior of our accumulation-mode devices. We also present comparisons to recently obtained experimental results on addition spectra in accumulation-mode quantum dots and show that our models correctly capture the relevant behavior. In addition, we address the robustness of device designs with respect to randomly distributed discrete dopants using a semi-analytical model and full numerical simulation based on impurity-induced random potentials.

4:18PM X17.00010 Si double quantum dot spin qubit in a MOSFET structure, QUIZI LI, DAMITRICE CULCER, LUKASZ CYWINSKI, SANKAR DAS SARMA, University of Maryland, College Park — Motivated by recent experimental developments, we theoretically consider the prospects for creating spin qubits in a lateral double-dot structure fabricated in a Si MOSFET by lithographic patterning. We calculate tunnel coupling, exchange splitting, and other relevant qubit properties as functions of the double-dot structural parameters, i.e. dot separation, central barrier, detuning, etc. Our motivation is to obtain a detailed qualitative comparison between GaAs and Si double-dot systems to see whether a Si MOSFET double-dot structure is feasible as a spin qubit in real quantum computer architectures. We will discuss both regular single electron spin qubit and the successful (in GaAs quantum dots) singlet-triplet spin qubits.

4:30PM X17.00011 Accumulation-Mode Quantum-Dot Devices, MATTHEW BORESELLI, EDWARD CROKE, MARK GYURE, ROBERT HAYES, IVAN MILOSAVLEVIC, ADELE SCHMITZ, JEONG-SUN MOON, ANDREW HUNTER, HRL Laboratories, LLC. — We have developed a quantum-dot device based on a double-well heterostructure in which electrons are localized in the top, mostly empty small circular gate. Charge occupancy changes in the dot are monitored by measuring current confined to a narrow channel in the bottom well. In this design, dot occupancy is primarily controlled by a single gate and interacting dots can be straightforwardly fabricated. We have successfully fabricated and characterized single-dot of devices of this design in AlGaAs/InGaAs, and are extending the design to SiGe/Si heterostructures. We have measured charging spectra of III-V versions of the device down to zero electron occupancy. Charging spectra show enhanced stability for n=2, 6, 12, and 20 electrons. We have measured the tunneling times as a function of bias to map out excited states of a two-electron dot.

4:42PM X17.00012 Cross-correlation heterodyne detection part I: Measuring the vacuum fluctuations at microwave frequencies, MATTEO MARIANTONI, EDWIN P. MENZEL, M. A. ARAQUE CABALLERO, F. DEPPE, E. HOFFMANN, T. NIEMCZYK, A. MARX, R. GROSS, Walther-Meissner-Institut and TU Muenchen, Germany, E. SOLANO, Departamento de Quimica Fisica, Universidad del Pais Vasco / Euskal Herriko Unibertsitatea, Spain — In order to gain a profound insight into the fundamental properties of quantum electrodynamics (QED), studying the zero-point fluctuations of microwave radiation represents an important task. Here, we present a full experimental characterization of the vacuum fluctuations by measuring the Planck distribution of its noise power at microwave frequencies and very low temperatures. We observe a cross-over from thermal noise to vacuum quantum noise and quantify the level of vacuum fluctuations for a narrow frequency band centered around 5.85 GHz. We demonstrate the change of the vacuum fluctuations level with the center frequency. Finally, we perform a new type of heterodyne detection particularly suitable for circuit QED systems. It is based on a new, homodyne, cross-correlation method. The latter allows for the reconstruction of the entire covariance matrix of the vacuum. We acknowledge support from SFB631, NIM, EuroSQUIP, and the Ikerbasque Foundation.


1Work supported by LPS-NSA

1Sponsored by United States Department of Defense. Approved for Public Release, Distribution Unlimited
In this contribution, we present our studies of Michelson and Fabry-Perot interferometers with WILDFEUER, LOUISIANA STATE UNIVERSITY, AARON J. PEARLMAN, JUN CHEN, Joint Quantum Institute, National Institute of Standards and Technology, and University of Maryland, JONATHAN P. DOWLING, Hearne Institute for Theoretical Physics, Louisiana State University, BATON ROUGE TEAM, Joint QUANTUM INSTITUTE, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, AND UNIVERSITY OF MARYLAND TEAM — In this contribution, we present our studies of Michelson and Fabry-Perot interferometers with a photon-number resolving detector. We show experimentally that with a weak coherent light beam, the use of a photon-number resolving detector improves the interferometric resolution. We also discuss ways the sensitivity of interferometers can be further improved beyond the standard quantum limit by using nonclassical light and photon-number resolving detectors.

Thursday, March 19, 2009 2:30PM - 5:30PM – Session X18 DPOLY: Elastomers and Gels I

2:30PM X18.00001 Phase behavior of poly(ethylene oxide) in ethyl alcohol / water mixtures, S. H. SHIN, R. M. BRIBER, University at College Park, B. HAMMOURDA, D. L-T HO, National Institute of Standards and Technology — PEO in ethanol forms an opaque gel-like mixture with a partial crystalline structure. Addition of a small amount of water disrupts the gel: 5% PEO in ethanol with the addition of 4-10% water becomethan as an athermal polymer solution and the phase behavior changes from UCST to LCST rapidly as the fraction of water is increased. The observed origin of this unusual phase behavior comes from the formation of a hydration layer around the PEO chain. Two water molecules can hydrate one PEO monomer which is consistent with the suppression in the crystallization and change in the phase behavior observed by SANS. We measured the spinodal temperature and phase behavior of PEO solutions with different concentrations of PEO (2% PEO and 10% PEO) in the mixed water/ethanol solvent system to assess the role of hydration. The observed phase behavior is consistent with a hydration layer forming upon the addition of water and the system shifting from UCST to LCST behavior. The amount of water necessary to form a hydration layer around PEO chains varies in a self-consistent manner as the PEO concentration increases from 2 to 10%.

2:42PM X18.00002 pH-Responsive Swelling of PAMAM Dendrimer-Gels, RONALD HEDDEN, BURCU UNAL, Penn State University — End-linked hydrogels containing high mass fractions of amine-terminated poly(amideamine) (PAMAM) dendrimers are prepared by reaction of dendrimers with monodisperse, epoxide-terminated linear poly(ethylene glycol) chains. PAMAM dendrimers impart pH-dependent swelling characteristics to the gels, which absorb large amounts of water due to protonation of the dendrimers' amine groups under neutral or weakly acidic conditions. The equilibrium swelling of the gels passes through a maximum at pH of approximately 4.5, due to extensive protonation of the amine groups. Interestingly, the equilibrium swelling ratio is marked lower at both high external pH and low external pH. We model the swelling behavior by invoking the Donnan equilibrium theory, treating the gels as phantom networks that contain a high concentration of Lewis bases having pHb=3.5. The model captures the maximum in swelling near pH=4.5, though equilibrium swelling ratio is overpredicted in some cases. The collapse of the gels at both high and low external pH is explained in terms of the differential between the concentrations of mobile ions inside and outside the gel. We will discuss recent attempts to prepare stimuli-responsive gels based upon the remarkable swelling characteristics of PAMAM dendrimer-gels.

2:54PM X18.00003 Studies on shear-thinning and recovery properties of beta-hairpin peptide hydrogel, CONGQI YAN, RADHIKA NAGARKAR, JOEL SCHNEIDER, DARRIN POCHAN, University of Delaware — In solution, freely soluble, unfolded MAXI peptide ((VK)2-V(2)PPT-(VK)4-CO-NH2) undergoes a conformation change into a folded/hairpin by exposure to a folding stimulus, e.g. pH change, salt addition, or temperature rise. The consequent self-assembly leads to a stiff hydrogel stabilized by physical crosslinks between fibrillar nanostructures. When a proper shear stress is applied, the hydrogel shear-thins and flows. Moreover, as soon as the stress is ceased, the gel immediately reheals into a stiff solid and recovers its original mechanical strength quickly. This shear-thinning and rehealing property makes possible hydrogel delivery via syringe injection. In this work, Rheo-SANS was adopted to monitor the gel network morphology under shear flow. Also, rheological experiments were performed to measure the gel recovery after shear-thinning under various shear treatment conditions. Laser scanning confocal microscopy was used to observe the flow and velocity profile of the hydrogel through a channel. The results explain morphology changes of the gel network during shear-thinning and subsequent rehealing process. The fundamental gel shear-thinning and rehealing mechanisms will be discussed.

3:06PM X18.00004 Poly(Z-Lysine)-based Block Copolymer Organogels, SANDEEP S. NAIK, ADAM D. RICHARDSON, DANIEL A. SAVIN, School of Polymers and High Performance Materials, University of Southern Mississippi — A series of AB diblock copolymers consisting of poly(Lysine)(Z) (A = P(Lys(Z))) and poly(propylene oxide) or polyhedral oligomeric silsesquioxane (B = PPO, POSS) were synthesized and found to form stable, rigid organogels in THF and chloroform at room temperature. In these systems, the protecting group on the P(Lys) side-chains remains intact. As such, the secondary structure of the polypeptide chains retains helicity over a wide range of solution conditions. Gel formation in these systems results from the assembly of the solventphobic P(Lys(Z)) chains, which pack densely in an anti-parallel fashion, minimizing interfacial curvature. These gels all exhibited shear-thinning behavior, and as the temperature was heated to 350 K exhibited a gel-sol transition. The role of solvent polarity and molecular weight of the P(Lys(Z)) chains on the mechanical strength will be discussed.
3:18PM X18.00005 Anisotropic Poly(Vinyl Alcohol) Hydrogel: Connection Between Structure and Bulk Mechanical Properties1, STEPHEN HUDSON, JEFFREY HUTTER, LEONARDO MILLON, WANKEI WAN, The University of Western Ontario, Canada, MU-PING NIH, National Research Council Canada — Poly(vinyl alcohol) (PVA) hydrogels are formed from PVA solution by cross-linking of physical cross-links through freeze/thaw cycling. By choosing a suitable freeze/thaw protocol and applying a strain during thermal processing, gels with permanent, anisotropic bulk mechanical properties matching those of cardiovascular tissues can be made, making them useful for applications ranging from artificial heart valves to vascular grafts. We have performed small- and ultra-small-angle neutron scattering (SANS and USANS) measurements covering length scales from 2 nm to 10 µm, and modeled the structure as interconnected PVA blobs of size 20 to 50 nm arranged in fractal aggregates extending to at least 10 µm. Here, we discuss the relationship between the microstructure and bulk mechanical properties. Strength increases with the number of thermal cycles due to reinforcement of the small-scale gel phase, while anisotropy is due to elongation of the much larger fractal aggregates.

1Supported by NSERC and AFMNet (Canada). This work utilized facilities supported by the Department of Commerce and NSF agreement DMR-0454672 (USA).

3:30PM X18.00006 Kinetics of phase separation of thermoreversible gels, FRANCISCO J. SOLIS, ASU West, CHRISTINE LEON, BRENT VERNON, Arizona State University — We study the kinetics of phase separation and thermoreversible gel formation of LCST-type polymers. A large number of NIPAM-based polymers exhibit transitions near room temperature from a liquid phase to a two-phase state. In the two-phase region of the phase diagram, a polymer dilute phase coexists with a gel. The corresponding shrinking transition for chemically-linked gels has been extensively studied in both its thermodynamic and kinetic aspects. We show that, in the thermoreversible case, the formation of the gel phase proceeds in a similar way. Upon entrance to the two-phase region, the gel volume follows a double exponential decay. The gel undergoes a fast shrinking associated with water ejection, followed by a slower reorganization regime.

3:42PM X18.00007 Structure and Rheology of Leucine Zipper Protein Hydrogels, B.D. OLSEN, J.A. KORNFIELD, D.A. TIRRELL, California Institute of Technology — Protein hydrogels from telechelic polymers physically crosslinked by the specific association of leucine zipper domains provide fundamental insight into polymer network structures due to the unparalleled control over molecular weight and network junction multiplicity. Two different leucine zippers are used to confer either tetrameric or pentameric end block association. By varying the length of the polyelectrolyte midblock, we show that the macroscopic and rheological properties of the hydrogels depend on both the polymer molecular weight and the aggregation state of the leucine zipper junctions. Cryo-TEM and negative staining are used together to visualize the gels, revealing heterogeneous structures. The gels are strongly shear thinning, and examination of Lissajous figures of stress vs. strain suggest a yielding mechanism. Under many conditions the gels can recover nearly their full strength less than a minute after the cessation of shear. These properties combined with the ease of biofunctionalization and pH and temperature responsive gelation transitions make the materials attractive for tissue engineering.

3:54PM X18.00008 Morphology of biaxially stretched triblock copolymer gels using SAXS, ARJUN KRISHNAN, TUSHAR GHOSH, RICHARD SPONTAK, North Carolina State University — Gels of styrenic triblock copolymers swollen by a low-volatility, midblock-selective oil behave as high-strain, low-field dielectric elastomers in the design of electroactive polymeric actuators. A standard configuration of such devices involves stretching, or “prestraining,” the elastomer film biaxially. However, little is known about the effect of biaxial prestrain on copolymer morphology. In this study, small-angle X-ray scattering (SAXS) is used to probe the nanostructure of gels composed of polystyrene-((ethylene-co-butylene)-(styrene) and mineral oil by systematically changing the concentration of polymer from 5 to 30 wt% and the biaxial prestrain from 0 to 300%. In the azimuthally integrated intensity profiles, the form factor due to scattering from polystyrene microdomains correlates strongly with polymer concentration and does not change with the applied prestrain, indicating that the polystyrene crosslinks remain as polystyrene spheres. The structure factor data correlates with prestrain, and is fitted using the Percus-Yevick approximation for interacting spheres. While a hard sphere interaction model is sufficient for unstrained gels, we resort to a square shoulder hard sphere potential for strained samples.

4:06PM X18.00009 Computer Simulation of a Switchable Metallo-Supramolecular Gel1, SHIHU WANG, ELENA DORIMONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University — Using Monte Carlo simulation, we studied reversible metallo-supramolecular gel comprised of linear oligomers end-functionalized with ligands and metal ions that can form trans- or cis-ligand-metal complexes with a ratio up to 3:1. We found that cis-isomers exhibit a larger overall degree of association and higher average molecular weight compared to trans-isomers due to a larger fraction of 3:1 or 2:1 ligand-metal complexes. Furthermore the metallo-supramolecular gel formed by cis-isomers occurs within a wider range of metal-to-oligomer ratios at a lower oligomer concentration and exhibits a larger elastic modulus and a smaller mesh-size compared to gel formed by trans-isomers. We found that exchanging cis-to-trans-isomers leads to a monotonic change of the material properties for most cases except for the 2:1 ligand:metal ratio at which the mesh size exhibits a minimum due to the favorable formation of intra-molecular bonds by cis-isomers. These switchable properties suggest interesting application opportunities.

1This work was supported by the NSF Career Award CHE-0348302.

4:18PM X18.00010 Cavitational Rheology and Fracture Behavior of Polyacrylamide Hydrogels, SANTANU KUNDU, ALFRED CROSBY, University of Massachusetts- Amherst — Cavitational rheology is a new characterization technique for the measurement of mechanical properties on small length scales, e.g. 10-1000 µm, at any arbitrary location within a soft material. The technique involves growing a cavity at the tip of a syringe needle and monitoring the pressure of the cavity at the onset of instability. This critical pressure is directly related to the local modulus of the material. We used this technique to characterize the network mechanics of polyacrylamide hydrogel materials, a common material used in many biological applications. Gels with different moduli, which were obtained by varying initial monomer to water ratio, were investigated. As monomer concentration increased, a transition from stable cavity to fracture was observed. Applying scaling theory for gels, we modify the Lake-Thomas Theory for the fracture of crosslinked networks to relate the transition from cavitational to fracture in terms of molecular parameters. We anticipate this fundamental understanding of cavitational and fracture mechanism will be applicable to biological tissues, as well as the development of advanced soft materials.

4:30PM X18.00011 Dynamic display of biomolecular patterns through an elastic creasing instability of stimuli-responsive hydrogel surfaces, JUNGWOOK KIM, RYAN HAYWARD, University of Massachusetts, Amherst — Swelling a soft hydrogel film attached to a rigid substrate generates a lateral biaxial compressive stress within the gel. For sufficiently large stresses, the free surface of the gel undergoes a mechanical instability to form sharp creases on its surface. We have taken advantage of this process using temperature-responsive hydrogels to fabricate dynamic scaffolds that reversibly hide and display biomolecular patterns. Desired bioactive ligands are grafted to polyelectrolytes, which are then selectively deposited to pattern the hydrogel surface. The shapes of the patterns are directed by topographic features of the underlying substrate. At room temperature, the functionalized areas of the surface are hidden within creases, but as the temperature is raised, dehydration of the gel leads to unfolding of creases and exposure of the biomolecular patterns. By switching on and off the patterns, we could engineer dynamic interactions between our scaffolds and target objects such as microscopic beads or cells.
hard segments. Ionic conductivity measurements reveal that the through-plane conductivity increases by an order of magnitude upon stretching. The characteristic spacing between the pseudo-cylindrical aggregates increases with the molecular weight of the PDMS segments and the size of the hard charged segments, that include DABCO. X-ray scattering patterns were recorded at the small, intermediate and wide angle regions for both un-stretched and stretched films. Stretching induces orientation without changing the spacing in the morphology. The hard charged segments, that include DABCO, align in pseudo-cylindrical aggregates in the direction of the stretch and the PDMS soft segments remain amorphous. The orientation relative to the stretching direction suggests that the hard charged segments induce orientation without changing the spacing in the morphology. The stable bonds between the nanogels play an essential role by forming a backbone that provides a mechanical strength to the material. The simulations show that just a relatively small fraction of such labile bonds (roughly 15%) are needed to prevent the catastrophic failure of the sample. The findings provide guidelines for creating high-strength, self-healing materials.

5:06PM X18.0014 Effect of Confinement on the Dynamics of Three-Dimensional Chemo-responsive Gels, OLGA KUKSENOK, VICTOR V. YASHIN, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — Chemo-responsive gels undergo the Belousov-Zhabotinsky (BZ) reaction could be ideal candidates for creating materials that can perform sustained mechanical work. We use theory and simulation to investigate the behavior of three-dimensional samples of BZ gels that are spatially confined in various geometric arrangements and show that the spatial confinement has a dramatic effect on the samples' dynamics. We first perform a linear stability analysis in two limiting cases, where a small sample is either completely free or attached at all the boundaries to fixed, hard walls. We find the critical reaction parameters at which the gels undergo a transition from a stationary steady state to an oscillatory regime in each of these cases. We then carry out corresponding computer simulations using our 3D gel lattice spring model and find an excellent agreement between the theory and simulations. Furthermore, we illustrate that the above analysis allows us to predict the behavior of larger samples that are confined in more complex spatial arrangements.

5:18PM X19.0015 Diffusion of molecular probes and proteins in hydrogels, RICCARDO RACCIS, ROBERT ROSKAMP, ANNETTE BRUNSEN, MAX PLANCK INSTITUTE FOR POLYMER RESEARCH, F.O.R.T.H. INSTITUTE OF ELECTRONIC STRUCTURE AND LASER TECHNOLOGY, WOLFGANG KNOLL, AUSTRIAN RESEARCH CENTERS, GEORGE FYTAS, MAX PLANCK INSTITUTE FOR POLYMER RESEARCH, F.O.R.T.H. INSTITUTE OF ELECTRONIC STRUCTURE AND LASER TECHNOLOGY — We employ fluorescence correlation spectroscopy to study the diffusion of molecular probes (Cy5) and dye-tagged proteins (Cy5-Ab-LlN21f, hydrodynamic radius 10nm and Alexa488-Streptavidin, 4nm) in surface-attached poly-N-isopropylacrylamide (PNIPAAm) gels. The diffusion process depends on the crosslinking density and the presence of electrostatic and steric interactions. The protein penetration into the hydrogel layer occurs close to the isoelectric point but the local probe concentration and diffusion rate diminish with increasing penetration depth. Mesh size characterization of the hydrogels is inferred from the diffusivity and the concentration profile of fluorescent probes with different size, with the molecular free dye diffusing deeper into the gel.

Thursday, March 19, 2009 2:30PM - 5:30PM Session X19 DPOLY: Charged and Ion-containing Polymers 320

2:30PM X19.0001 Molecular Weight and Charge Density Asymmetry in Polyelectrolyte Complexation, DEBRA AUDUS, GLENN FREDRICKSON, University of California, Santa Barbara, DOMINIJK DUECHS, Max Planck Institute, Mainz — We investigate the phase diagram of oppositely charged polymers in a good solvent using a field-theoretic model. Mean-field solutions fail to predict the experimentally observed macroscopic phase separation into a solvent-rich phase and a dense liquid aggregate of polymers - a “complex coacervate.” We therefore study the model within a one-loop approximation, which accounts for Gaussian fluctuations in electrostatic and chemical potentials. Our particular focus is the effect of molecular weight, ionic strength, and charge asymmetry on the phase envelope. A set of dimensionless parameters is identified that dictate the size and shape of the two-phase region. Our results should be helpful in guiding experimental studies of coacervation.

2:42PM X19.0002 PEG-based Sulfonated Ionomers Microphase Separate with Increasing Temperature, WENQIN WANG, Department of Materials Science and Engineering, University of Pennsylvania, GREGORY J. TUDRYN, RALPH H. COLBY, Department of Materials Science and Engineering, Pennsylvania State University, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — A series of Li, Na, and Cs-neutralized sulfonated polymer ionomers with well-defined PEG spacer lengths have been investigated by in situ X-ray scattering over a wide temperature range. At room temperature, no “ionomer peak” at q ~1-5 nm^-1 was observed, due to the high dielectric constant of the polymer matrix. As the length of the PEG segment increases, the crystallization of PEG segments is evidenced by multiple crystalline reflection peaks. In addition, crystallization produces periodic low-angle peaks, indicating a layered structure. Scanning transmission electron microscopy will be employed to predict the behavior of larger samples that are confined in more complex spatial arrangements.

2:54PM X19.0003 Hierarchical Structures in PDMS-based Ammonium Ionomers, DAVID SALAS-DE LA CRUZ, University of Pennsylvania, SUDIPTO DAS, GARTH WILKES, Virginia Tech, KAREN WINEY, University of Pennsylvania — Ionomers are polymers with a charged entity in a backbone. Polyethylene (PE) and ionomers were synthesized from 6-monomer poly chloride and 1,4-diazabicyclo[2.2.2]octane (DABCO). X-ray scattering patterns were recorded at the small, intermediate and wide angle regions for both un-stretched and stretched films. Stretching induces orientation without changing the spacing in the morphology. The hard charged segments, that include DABCO, align in pseudo-cylindrical aggregates in the direction of the stretch and the PDMS soft segments remain amorphous. The orientation relative to the stretching direction suggests that the hard charged segments self assemble into anisotropic aggregates. This self-assembly arises from the hydrogen bonding of the urethane groups and ion sharing between Br^- and N+. The characteristic spacing between the pseudo-cylindrical aggregates increases with the molecular weight of the PDMS segments and the size of the hard segments. Ionic conductivity measurements reveal that the through-plane conductivity increases by an order of magnitude upon stretching.
Temperature and pH Responsive Chargeable Copolymers with Tunable LCSTs, KIATTIKHUN MANOKRUANG, EVANGELOS MANIAS, Materials Sci & Eng; Penn State University — A series of alternating copolymers, made of \( \alpha, \omega \)-polyethylene glycol oligomers (M\(_\text{w} \)= 400 or 900) alternating with 1,6-diamino-hexane-star-lysine, is presented. Specifically their aqueous phase behavior is outlined, exhibiting temperature-controlled solubility (LCST) and a pH-controlled transition (across the point where lysine is charged). The terpolymers are uncharged at low pH while they become charged (containing lysine anions) when the solution pH increases; the phase diagrams in the temperature and pH space are drawn, and the tunability of the critical points in water as it is controlled by the copolymer composition is discussed. These copolymers, due to their hydrophilic polyethylene-oxide comonomers, exhibit a genuine LCST, i.e., a bona fide first order thermodynamic transition, rather than the usual micellization related LCST of copolymers that contain hydrophobic blocks or grafts. This last point is demonstrated by comparisons against micelle-forming copolymers, consisting of hydrophobic and chargeable comonomers.

Ionic Conductivity of Poly(ethylene oxide)-Containing Block Copolymers at Order-Disorder and Order-Order Transitions, NISITA WANAKULE, UC Berkeley, ASHOUTOSH PANDAY, SCOTT MULLIN, NITASH BALSARA, UC Berkeley, Lawrence Berkeley National Labs — The order-disorder transition (ODT) and order-order transition (OOT) of block copolymers with lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salts are measured with a combination of small-angle x-ray scattering (SAXS) and birefringence. The block copolymers comprise of polyethylene oxide (PEO), a polymer with a higher dielectric constant that dissolves LiTFSI, and polystyrene (PS), a polymer with a lower dielectric constant that does not dissolve LiTFSI. Ionic conductivity of the block copolymers is measured through the observed ODT and OOT. The effect of morphology on the ionic conductivity will be presented and compared with literature results.

Origin of Lateral Nanoscale Heterogeneities in Weak Polyelectrolyte Brushes, YOU-YEON WON, KEVIN WITTE, JAEHYUN HUR, Purdue University — In this talk, we will first discuss experimental evidence of lateral nanoscale heterogeneities in a single-component weak polyelectrolyte brush system under zero to low salt conditions. Using an amphiphilic diblock copolymer, poly(2-(dimethylamino)ethyl methacrylate-b-n-butyl acrylate) (PDMAEMA-PnBA), for Langmuir film compression and Langmuir-Blodgett deposition on a hydrophobic substrate followed by fluid AFM imaging, we show the existence of regions of different brush heights, indicative of the thermodynamic instability (and resultant local clustering) of the PDMAEMA chains in the low-salt limit. Using SCF and scaling theories, we will also show that the lateral heterogeneities occur due to the combined effects of (i) the osmotic instability regulated by charge equilibrium and (ii) the hydrophobicity of the chains.


Counter-ion fluctuations in the presence of a spherical macromolecule, LEANDRO BOONZAEBER, KRISTIAN K. MUELLER-NEDEBOEK, Institute of Theoretical Physics, University of Stellenbosch, 7600 Matieland, South Africa, FREDERIK G. SCHOLTZ, National Institute for Theoretical Physics, Stellenbosch Institute for Advanced Study, 7600 Stellenbosch, South Africa — The effective interactions of charged macromolecules (e.g. polyelectrolytes) are still not fully understood. The role of counter-ion fluctuations, in the presence of these macromolecules, seems to be crucial in understanding these effective interactions. We consider a single charged spherical macromolecule, enclosed in a finite volume, in the presence of point-like counter-ions in an electrically neutral solution. Writing the partition function as a functional integral and only keeping terms up to quadratic order, we calculate the free energy in this approximation exactly.

Counterion Condensation and Collapse of Sodium Polystyrene Sulfonate in Water: A Molecular Dynamics Study, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Hydrophobic polyelectrolytes are known to form necklace-like structures of dense beads connected by strings of monomers. This structure appears as a result of optimization of electrostatic and short-range interactions. To elucidate the effect of counterion condensation on polyelectrolyte conformations we performed two sets of molecular dynamics simulations of sodium polystyrene sulfonate (NaPSS) chains with degree of polymerizations \( N=16, 32 \) and 64 and fraction of charged monomers \( f=0.25, 0.33, 0.5 \) and 1.0 in aqueous solutions; (1) water molecules were considered explicitly using TIP3P model and (2) water molecules were modeled as a dielectric continuum with dielectric constant 77.73. Our simulations showed that with increasing \( f \) a polyelectrolyte chain adopts an elongated conformation. The transition between collapsed and elongated states does not show any features of abrupt transition due to the fact that only relatively short chains were considered. Furthermore, even for our longest chains (\( N=64 \)) the necklace-like globule was not observed. Effect of the water-ion interactions on counterion condensation was analyzed by comparing the radial distribution function between the sulfonate groups and sodium counterions for chains with different \( f \). It was found that in simulations with explicit water ionized groups are located at the globular surface.
is also apparently important. Within the film (quantified by neutron reflectivity measurements) can have a large effect on the surface morphology diagram and the physics of glass-formation (flow coated versus spun cast films) so non-equilibrium effects evidently have a large effect on the surface pattern morphology. In particular, the residual solvent and we construct a surface morphology diagram as a function of hf and T. The surface morphology diagram is found to depend on the method of film formation cylinders oriented parallel to the substrate to a mixed or 'hybrid' state where the two orientations coexist (b) this hybrid morphology then transforms to cylinders with both blocks. Surface morphology transitions with increasing hf are observed in these model 'frustrated-interaction' films: (a) first, a transition occurs from increasing hf when the substrate interaction is highly selective for one of the blocks (PMMA) and the polymer-air interface has a nearly neutral interaction block-methyl methacrylate) (PS-b-PMMA). A transition from a perpendicular to a parallel cylinder orientation with respect to the substrate is observed upon the addition of external salts, the hydrodynamic radius of PSSNa was found to decrease with the increase of salt concentration, i.e., the chain contracts due to electrostatic screening and ion bridging effect. When the salt concentration increased beyond a certain value, the chains were observed to increase their dimension for a mono-, double- and triple-valent counterions. The experimental evidence shows the single chain behavior of re-entrant transition of polyelectrolytes.

1Project supported by National Natural Science Foundation of China (NSFC).

4:06PM X19.00014 Single chain contraction and re-expansion by counterions of polyelectrolytes 1. FENGXUANG JIA, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — We have studied the re-entrant transition of polyelectrolytes at single chain level. Diffusion rate of single chains of polystyrene sulfonate (PSSNa) has been investigated by fluorescence correlation spectroscopy under different counterion condition. Upon the addition of external salts, the hydrodynamic radius of PSSNa was found to decrease with the increase of salt concentration, i.e., the chain contracts due to electrostatic screening and ion bridging effect. When the salt concentration increased beyond a certain value, the chains were observed to increase their dimension for a mono-, double- and triple-valent counterions. The experimental evidence shows the single chain behavior of re-entrant transition of polyelectrolytes.

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Thursday, March 19, 2009 2:30PM - 5:30PM – Session X20 DPOLY: Long Range Order in Polymer Structures and Morphologies

2:30PM X20.00001 Long range ordering in block copolymer thin films. CAROLINE ROSS, MIT — Thin films of microphase separated block copolymers, which can form patterns consisting of dense arrays of lines or dots, are attractive materials for self-assembled nanoscale lithography. The long range order of the block copolymer microdomains can be controlled by the use of chemical or topographical patterns. In this work, we discuss how Si-containing block copolymers, polystyrene-b-polyferrocenylidimethylsilane (PS-PFS) and polystyrene-b-polydimethylsiloxane (PS-PDMS), can be templated on substrates patterned with posts or steps. In the case of 40 nm period spherical morphology PS-PDMS, <20 nm diameter posts, which are coated with a grafted layer of PDMS homopolymer, define the locations of surrounding PDMS microdomains. The lattice spacing and orientation of the templated PDMS microdomain array can be predicted from the ratio between the post spacing and the equilibrium microdomain spacing. PFS spheres, formed from spherical-morphology PS-PFS, can be aligned within shallow trenches to form a close-packed array with row spacing determined by the trench width. We also show how 32 nm period cylindrical morphology PS-PDMS can be templated using topographical features. Templating using posts or linear substrate features gives arrays of straight parallel cylinders with controllable period and orientation, while templating in circular pits creates sharply curved, concentric toroidal structures. The overall morphology and period of the block copolymer microdomain arrays can be varied by solvent annealing in mixed solvent vapors, for example cylindrical-morphology PS-PDMS can form perforated lamellae by annealing in toluene plus heptane. These results will be discussed in the context of nanolithography, including examples of pattern transfer to form metal, oxide and polymer functional nanostructures. Bita et al, Science 321 939 (2008); Jung et al, Nano Letts. 7 2046 (2007); 8 2875 (2008).

3:06PM X20.00002 Surface Morphology Diagram for Cylinder-Forming Block Copolymer Thin Films. ALAMGIR KARIM, University of Akron, XIAOHUA ZHANG, JACK DOUGLAS, RONALD JONES, Polymers Division, NIST — We investigate the effect of annealing temperature (T) and film thickness (hf) on the surface morphology of flow coated films of a cylinder forming block copolymer, poly (styrene-block-methyl methacrylate) (PS-b-PMA). A transition from a perpendicular to a parallel cylinder orientation with respect to the substrate is observed upon increasing hf when the substrate interaction is highly selective for one of the blocks (PMMA) and the polymer-air interface has a nearly neutral interaction with both blocks. Surface morphology transitions with increasing hf are observed in these model ‘frustrated-interaction’ films: (a) first, a transition occurs from cylinders oriented parallel to the substrate to a mixed or ‘hybrid’ state where the two orientations coexist (b) this hybrid morphology then transforms to cylinders oriented perpendicularly to the polymer-air interface for larger hf. The characteristic values of hf defining these surface morphological transitions depend on T and we construct a surface morphology diagram as a function of hf and T. The surface morphology diagram is found to depend on the method of film formation (flow coated versus spin cast films) so non-equilibrium effects evidently have a large effect on the surface pattern morphology. In particular, the residual solvent within the film (quantified by neutron reflectivity measurements) can have a large effect on the surface morphology diagram and the physics of glass-formation is also apparently important.
3:18PM X20.00003 Practical Implementation of Order Parameter Calculation for Directed Assembly of Block Copolymer Thin Films.

The use of the Advanced Light Source, Berkeley National Laboratory, supported by the U.S. Department of Energy, Office routes to ultrahigh density, addressable systems. The sawtoothed substrate topography provides registered, directional guidance of the BCP self-assembly that is tolerant of surface defects, maintaining the application of these parameters and analyze with a high level of accuracy the translational and orientational parameters of the guiding pattern, the domains of a block copolymer directed to assemble on this pattern, as well as the underlying structure after lift-off. We observe that order can be preserved over a large area and can be retained in subsequent processing.

3:30PM X20.00004 Controlling the self-assembly of block copolymer materials in thin-films.

UNYONG JEONG, Dept. of Metallurgical Engineering, Yonsei University, TING XU, Dept. of Materials Science and Engineering, University of California, PARK, DONG HYUN LEE, BOKYUNG KIM, SUNG WOO HONG, JI XU, Dept. of Polymer Science and Engineering, University of Massachusetts Amherst, EUNGNAK HAN, Department of Materials Science & Engineering, University of Wisconsin-Madison, KARL STUEN, PAUL NEALEY, Department of Chemical & Biological Engineering, University of Wisconsin-Madison, PADMA GOPALAN, Department of Materials Science & Engineering, University of Wisconsin-Madison — We present a simple and efficient strategy towards surface modification for controlling the self-assembly of P(styrene-b-methylmethacrylate) diblock copolymer (BCP) in thin films. Photo-patternable, substrate-independent neutral surface was created to achieve vertical orientation of block copolymer (BCP) microdomains. A random copolymer of styrene (f= 0.58±0.03), methylmethacrylate (f= 0.41±0.06) and glycidyl methacrylate (f= 0.01±0.02) was synthesized. The copolymer uses photo-crosslinking reaction of epoxy groups by photoinitiator generator to formulate the neutral surface. Ultra-thin (2-6 nm) crosslinked film was created as a neutral interfacial layer between the block copolymer and the substrate. The composition of the copolymer was fine tuned to tailor the wetting behavior and hence the domain orientation (parallel or perpendicular to the substrate) in the self-assembled block copolymer film. The effectiveness of the new neutral polymer on a range of substrates such as glass and gold coated silicon wafer and for both symmetric and asymmetric BCPs is demonstrated.

3:42PM X20.00005 Shear Alignment and Realignment of Cylinder-Forming Block Copolymer Thin Films.

VINDHYA MISHRA, Materials Research Laboratory, University of California, Santa Barbara, EDWARD KRAMER, Department of Materials and Chemical Engineering, University of California Santa Barbara, SU-MI HUR, GLENN FREDRICKSON, Materials Research Laboratory, University of California, Santa Barbara, MICHAEL SPRUNG, Argonne National Lab, IL — In multilayer thin films of spherical morphology block copolymers, the surface layers prefer hexagonal symmetry while the inner layers prefer BCC. Thin films with spherical morphology of PS-b-P2VP blends with short homopolymer polystyrene (hPS) chains have an HCP structure up to a thickness n* at which there is a transition to a face centered orthorhombic structure. Using grazing incidence small angle X-ray scattering and transmission electron microscopy we show that that n* increases from 5 to 9 with increase in hPS from 0 to 12 vol%. For thicknesses just below n* the HCP and FCO structures coexist, but on long annealing HCP prevails. We hypothesize that the PS segregates to the interstices in the HCP structure reducing the stretching of the PS blocks and the free energy penalty of HCP versus BCC inner layers. Self consistent field theoretic simulations are being carried out to see if this idea is correct.

3:54PM X20.00006 Structural transition with thickness in films of poly-(styrene-2vinylpyridine) (PS-b-P2VP) diblock copolymer/homopolymer blends.

CHUANBING TANG, ERIN LENNON, MICHAEL DIMITRIOU, GLENN FREDRICKSON, EDWARD KRAMER, CRAIG HAWKER, Materials Research Laboratory, University of California, Santa Barbara — We present a modular and hierarchical self-assembling strategy for the generation of novel nanoscale patterns suitable for block copolymer lithography. Supramolecular block copolymers consisting of poly(ethylene oxide)-b-poly(styrene-4-vinylpyridine) and poly(styrene-2-vinylpyridine)-b-poly(methyl methacrylate) diblock copolymer blends with hydrogen-bonding interactions between the polystyrene majority segments were prepared by living free radical polymerization. By combining supramolecular assembly of H-bonding phenolic and pyridyl units with controlled phase separation of diblock copolymers, highly ordered square arrays were obtained. The compositions of H-bonding components were critical for generating both long range order and for controlling the spatial arrangement of ordered arrays. The utilization of these materials as lithographic masks was successful and allowed transfer of the polymeric template with high fidelity to silicon oxide substrates, leading to a highly ordered array of 20 nm cylindrical pores with a spacing of 50 nm. This modular blending approach to block copolymer resists demonstrates a new and powerful strategy for the fabrication of unique patterns for nanolithographic applications.


VINCENZO MEI, RICCARDO RUIZ, Hitachi Global Storage Technologies, San Jose Research Center, NICOLA FERRIER, Dept of Mech Engineering, University of California, Berkeley, THOMAS P. RUSSELL, Dept. of Polymer Science and Engineering, University of Massachusetts Amherst — We present a modular and hierarchical self-assembling strategy for the generation of novel nanoscale patterns suitable for block copolymer lithography. Supramolecular block copolymers consisting of poly(ethylene oxide)-b-poly(styrene-4-vinylpyridine) and poly(styrene-2-vinylpyridine)-b-poly(methyl methacrylate) diblock copolymer blends with hydrogen-bonding interactions between the polystyrene majority segments were prepared by living free radical polymerization. By combining supramolecular assembly of H-bonding phenolic and pyridyl units with controlled phase separation of diblock copolymers, highly ordered square arrays were obtained. The compositions of H-bonding components were critical for generating both long range order and for controlling the spatial arrangement of ordered arrays. The utilization of these materials as lithographic masks was successful and allowed transfer of the polymeric template with high fidelity to silicon oxide substrates, leading to a highly ordered array of 20 nm cylindrical pores with a spacing of 50 nm. This modular blending approach to block copolymer resists demonstrates a new and powerful strategy for the fabrication of unique patterns for nanolithographic applications.

4:18PM X20.00008 Macrosopic Addressable Arrays of Block Copolymer Microdomains.

The use of these materials as lithographic masks was successful and allowed transfer of the polymeric template with high fidelity to silicon oxide substrates, leading to a highly ordered array of 20 nm cylindrical pores with a spacing of 50 nm. This modular blending approach to block copolymer resists demonstrates a new and powerful strategy for the fabrication of unique patterns for nanolithographic applications.

This work was supported by the U.S. Department of Energy (DOE), the NSF supported MRSEC and NSEC at the University of Massachusetts Amherst. Use of the Advanced Light Source, Berkeley National Laboratory, supported by the U.S. Department of Energy, Office.
4:30PM X20.00009 Self-Extinguishing Crystallization: Copolymer Behavior under Flow , DIANA SMIRNOVA, MEISAM HAJIMORAD, JULIA KORNFIELD, California Institute of Technology — It is known that short chain branches in copolymers act as crystal defects, resulting in materials with low crystallinity and poorly-defined morphology. We are interested in the behavior of copolymers under flow in the presence of species that readily form well-defined shish-kebab morphologies. Bimodal blends containing small concentrations of high molecular weight, high density polyethylene (HDPE, Mw = 526 kg/mol, Mw/Mn = 3) in an ethylene-co-hexene matrix (Mw = 50 kg/mol, Mw/Mn = 2, 5 mol % hexene) were studied via rheo-optical and rheo-xray techniques. HDPE concentrations were selected above and below the overlap concentration of 0.6%, but maintained below 1% such that the rheology of the blends was not significantly altered from that of the copolymer matrix. DSC traces were collected to ensure that co-crystallization between the two blend components occurs. Crystallization after shear quickly leveled off revealing a self-extinguishing behavior. The time frame for this extinction is coupled with a loss of anisotropy in scattering patterns indicating random crystallization uncorrelated with existing oriented structures.

4:42PM X20.00010 Quasicrystalline long-range order in an ABC star block copolymer , TOMONARI DOTERA, Department of Polymer Chemistry, Kyoto University, Japan — We report the formation of a dodecagonal quasicrystal (DDQC) in a lattice Monte Carlo simulation of a star-shaped three component polymeric alloy. We have observed a series of Archimedean and quasicrystalline phases (4.82 \rightarrow (3^2.4.3.4) \rightarrow DDQC - (4.6.12) with increase of one component of ABC star polymers. This phase behavior can be regarded as a transition from square tilting to triangle tilting via square-triangle tilting. The simulation is associated with the recent striking experimental manifestation of quasicrystalline order: A mesoscopic tiling pattern with twelvefold symmetry in a three-component star polymer system composed of polyisoprene, polystyrene, and poly (2-vinylpyridine). Since, the same kind of quasicrystalline structures have been found for metal alloys, chalcogenides, and liquid crystals, the present result confirms the universal nature of quasicrystalline long-range order over several hierarchical length scales.


5:06PM X20.00012 Ligand-induced order in Spotted vesicles and Striped micelles , DAVID CHRISTIAN, WOUTER ELLENBROEK, ANDREA LIU, DENNIS DISCHER, MRSEC, University of Pennsylvania — Thermoplastic Polyurethanes (TPU) are linear block copolymers typically constructed of statistically alternating soft (SS) and hard (HS) segments. Due to their numerous industrial applications these materials have received considerable attention. We have investigated the phase behavior and morphology of a set of high hard block content polyurethanes and varied the chain extender used. Using mainly calorimetry, scattering and microscopy techniques we were able to elucidate the origins of all the thermal events observed through differential scanning calorimetry. Correlating our thermodynamic work with our structural work we were able to propose a new morphological model of the structure and the phase behavior of high hard block content polyurethanes. We have shown that above 65% hard segment content the melt-quenched samples present a two-phase morphology one pure hard segment phase co-existing with a mixed phase with the same hard segment content of 65% for all samples. When annealed at high temperature the mixed phase undergoes phase separation resulting in the same phase-separated mesophase. Changing the chain extender has a significant impact on the phase behavior and morphology of these systems

5:18PM X20.00013 Electrospinning of semicrystalline polymer fibers , YING LIU, Stony Brook University, SHUANG CHEN, CHUNHUA LI, ELAINE DIMASI, Brookhaven National Laboratory, GAD MAROM, The Hebrew University of Jerusalem, MIIRIAM RAFAILOVICH — Electro spinning of polymeric fibers has been attracted increased interest in recent years. However, the research for ethylene-vinyl acetate (EVA) and linear polyethylene (PE) is still limited, due to their relatively poor solubility in conventional solvent systems at ambient temperature. In this study, EVA and PE fibers were electro spun with different fiber diameter when the electro spinning solution was kept at a temperature greater than that of the solidification temperature of the polymer solutions. The effects of the fiber physical dimension to its crystallization and mechanical properties were thus detected. The morphology of the fibers was measured by scanning electron microscope (SEM) and atomic force microscope (AFM). The shear modulation force microscopy technique (SMFM) was used to measure the melting point, Tm, which was found to increase with increased fiber diameter and crystallinity. AFM three-point bending test demonstrated that the Young’s modulus of the fibers drastically increased as fiber diameter decreased. Grazing-incidence small angle x-ray scattering (GISAX) showed that, compared to the bulk material, the crystallinity of the electro spun fibers had been changed.

Thursday, March 19, 2009 2:30PM - 5:30PM
Session X21 FLAP DCMP: Spectroscopic Studies of Semiconductor Structure and Their Growth

2:30PM X21.00001 Electronic structure of Na_xCoO_2 investigated by X-ray absorption spectroscopy with Ab initio calculation , PAO-AN LIN, JIUNN-YUAN LIN, BEN HSU, HORNG -TAY JENG, CHEN-SHIUNG HSUE, YIA-CHUNG CHANG — The soft X-ray absorption spectra (XAS) of Na_xCoO_2 revealed marked and puzzling polarization dependence. It can not be explained by the degeneracy of \( e_g \) states generally believed in Na_xCoO_2. We fabricated the thin films of \( x = 0.68 \) and \( x = 0.75 \) to investigate the polarization dependence of XAS. Within the first principles DFT calculations, we have explanations for this phenomenon. After the analysis of the DOS of Na_xCoO_2, we presume that the pre-edge peaks at 529 eV and 530 eV of Na_xCoO_2 O-K edge may be not solely due to the unoccupied states of Co3+ and Co4+ eg states, but also due to the spacial asymmetry in the occupied Co 3d orbitals. Due to the hybridization between Co 3d & O 2p orbitals, the \( p_{x,y} \) and \( p_z \) states will be non-degenerate.

1This work was supported by the National Science Council and Academia Sinica, Taiwan. We also thank NCHC, CINCNUT, and NCTS for technical support
2:42PM X21.00002 Investigations of individual quantum dots of InAsP in InP nano-wires. MATS-ERIK PISTOL, NIKLAS SKÖLD, KIMBERLEY DICK, Lund University, CRAIG PRORY, University of Iowa, JACOB WAGNER, Danish Technical University, LARS SAMUELSON, Lund University — We have grown InP quantum wires containing InAsP quantum dots by metal-organic vapor phase epitaxy. These structures were investigated by transmission electron microscope and photoluminescence spectroscopy and were modelled by six-band k-p theory. We observe sharp emission lines from excitons, bi-excitons and tri-excitons. When we observe tri-exciton emission we observe lines originating from the s-shell as well as from the p-shell. By changing the size of the dots we observe clear confinement effects. The wires have a wurtzite structure but were modelled (by necessity) using zinc-blende parameters. From the deviation between the theory and the experiments we can deduce rough values of the band-gap of the wurtzite InAs as well as the electron effective mass of wurtzite InAs.

2:54PM X21.00003 Size dependent exciton g-factor in self-assembled InAs/InP quantum dots. PAUL KOENRAAD, NIEK KLEEMANS, JOOST VAN BREE, MURAT BOZKURT, ANDREI SILOV, RICHARD NOTZEL, Eindhoven University of Technology, CRAIG PRORY, MICHAEL FLATTE, University of Iowa — We have studied the size dependence of the exciton g-factor in self-assembled InAs/InP quantum dots. Photoluminescence measurements on a large ensemble of these dots indicate a multimodal height distribution. Cross-sectional Scanning Tunneling Microscopy measurements have been performed and support the interpretation of the macro photoluminescence spectra. More than 160 individual quantum dots have systematically been investigated by analyzing single dot magnetoluminescence between 1200nm and 1600 nm. We demonstrate a strong dependence of the exciton g-factor on the height and diameter of the quantum dots, which eventually gives rise to a sign change of the g-factor. The observed correlation between exciton g-factor and the size of the dots is in good agreement with calculations. The results demonstrate that quantum dots emitting at 1.55 micrometer and showing no Zeeman splitting (g-factor = 0) can be constructed. This makes these dots interesting for quantum information processing at optical telecommunication wavelengths.

3:06PM X21.00004 Optical and Electrical Characterization of Melt-Grown Bulk Ternary In$_x$Ga$_{1-x}$As 1. J. WEI, S. GUHA, L. GONZALEZ, Air Force Research Laboratory, P. DUTTA, G. RAJAGOPPLAN, United Semiconductors, Y. K. YEÖ, R.L. HENGEHOLD, Air Force Institute of Technology — Recent crystal growth technology breakthroughs led to successful growth of good quality bulk melt-grown ternary In$_x$Ga$_{1-x}$As single crystals. However, these bulk materials have not been well investigated compared to the epitaxial layers grown on a binary compound semiconductor, GaAs. Therefore, the optical and electrical properties of the bulk grown In$_x$Ga$_{1-x}$As have been investigated systematically as a function of temperature and In mole fraction $x$. The results show that the refractive index increases linearly with temperature from 100 to 300 K and also with In composition $x$ from 0.0 to 0.9 for several IR wavelengths. Typical refractive index values are 3.388 and 3.376 for 4.6 and 10.6 $\mu$m, respectively, at 300 K for $x$=0.5. The results of Hall-effect measurements show that the electron concentrations increase monotonically with $x$, while the mobilities decrease as $x$ increases from 0.5 to 1.0. Typical electron concentration and mobility at 300 K are $1.3\times10^{16}$/cm$^3$ and 9.1$\times10^3$/cm$^2$/V S, respectively, at $x$=0.75.

1 This work was partially supported by Air Force Office of Scientific Research.

3:18PM X21.00005 ABSTRACT WITHDRAWN —

3:30PM X21.00006 Structural, Optical and Electrical Properties of Sputtered InGaN Alloy Thin Films. MOHAMMAD EBDAH, DANIEL HOY, JOEL VAUGHN, MARTIN KORDESCH, Ohio University, DEPARTMENT OF PHYSICS TEAM — Amorphous and polycrystalline InGaN alloy thin films were successfully fabricated using rf sputtering technique with a sputtering targets of metal In and Ga in pure Nitrogen. Films were deposited on Si and quartz substrates, with the ratio of In to Ga being varied from 0 to 1 in the alloy. Growth under different sputtering conditions has been examined, such as different temperatures, pressures, and substrate-target distances. The corresponding obtained structures have been studied using the x-ray diffraction (XRD) and transmission electron microscope (TEM) techniques. The compositions have been verified by means of energy dispersive x-rays (EDX) spectroscopy and Rutherford back scattering (RBS). Multiple crystallographic phases have been investigated upon growth at different temperatures, and the existence of Gallium Nitride (GaN) and Indium Nitride (InN) phases were investigated. Hall effect measurements were made in 0.55 T magnetic field for characterizing the electrical resistivity at room temperature and 77 K, the free carrier concentration, and mobility. The optical bandgap and optical properties were studied by spectrophotometric and spectroscopic ellipsometric (SE) techniques.

3:42PM X21.00007 Atomic and electronic structure of AlN polar surfaces 1. MAOSHENG MIAO, ANDERSON JANOTTI, CHRIS VAN DE WALL, Materials Department, University of California, Santa Barbara — We studied the stability and electronic structure of AlN (0001) and (000-1) polar surfaces using first-principles DFT methods. A plane-wave basis set and PAW potentials are employed surface calculations. In order to correct the band gap of AlN, we applied the hybrid functional in the HSE [1] framework. Using this approach, we obtained a band gap of 6.1 eV, and lattice constants in excellent agreement with experimental values. Under Al-rich conditions, the Al adatom at T4 sites on the Al-terminated (0001) surface was found to be the most stable (2x2) reconstruction. This reconstruction is characterized by occupied surface states (Al dangling bonds) at 3.0 eV below the conduction-band minimum (CBM) and unoccupied surface states (Al dangling bonds) at 1.1 eV below the CBM. Under Al-poor conditions, the N adatom at the H3 site is the most stable reconstruction, with occupied N-Al bonding states at 4.2 eV and an unoccupied N-Al bonding state at 1.1 eV below the CBM. For the N-terminated (000-1) polar surface, the structure with an Al adlayer is the most stable under Al-rich conditions. The impact of the surface states on the properties of materials and devices will be discussed. [1] J. Heyd, G.E.Scuseria, and M. Ernzerhof, J. Chem. Phys. 118, 8207(2003).

1 ONR Award Number N00014-08-1-0095

3:54PM X21.00008 Micro-RDS to explore the spatial strain distribution in epitaxial AlN layers. CHUNHUA WANG, ZHIYU YANG, ZHIOQANG YAO, WENJUN ZHANG, DEPARTMENT OF PHYSICS, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM — A non-destructive method to observe the spatial resolved strain distribution in the sub-micrometer scale has been developed. By using micro-RDS to obtain the RA distribution on AlN films grown on Si and sapphire substrates, combining with the relation of the strain and optical anisotropy, we reveal the local strain distribution in the sub-micrometer scale. Strain domains several micrometers in size have been observed in AlN films grown epitaxially on Si without the amorphous interface layer. Each domain consists of hundreds of AlN grains. In films with many defects or grown on sapphire substrate there are no domains of dominant sizes, and the average strain is about 6 times smaller than the ones without the interface layer. The magnitude of the strain agrees well with the experimental values from the established methods such as XRD, TEM and Raman scattering.
of temperature. We will discuss possible mechanisms for persistent photoconductivity in these In...neighbors. Also, we observed distinct changes in the optical absorption spectra. Also, we studied the decay of the charge carrier density to the pre-illuminated state as a function...n...thin films. These films were grown on sapphire substrate by RF sputtering. Hall effect measurements carried out to measure the carrier concentrations, MI 48201, I.A. AVRUTSKY, Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI 48201, ALEXANDER EFROS, Center...RAGHAVAN PANGULURI, A. DIXIT, C. SUDAKAR, P. KHAREL, PUSHKAL THAPA, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, ALEXANDER EFROS, Center...D.M. NEWNS, IBM T. J. Watson Research Center, S. RAOUX, IBM Almaden Research Center, D.B. SHREKENHAMER, D.N. BASOV, UCSO, M.H. MUSER, U. of Western Ontario, D.M. NEWNS, IBM T. J. Watson Research Center — Phase change materials are materials that can be thermally interconverted between metallic (crystalline) and semiconducting (amorphous) phases. The interconversion process involves a change in local coordination number in some of the atomic constituents in these typically multicomponent materials. The electronic basis for the interconversion is still controversial. Here we report, in contrast to previous views, that the amorphization process is driven by an electronic reorganization in which lowering of the total energy by opening a Peierls-like gap drives the structural reorganization in the amorphous state, thereby explaining both the formation and semiconducting character of the amorphous phases. Our understanding of the process is based on phase transformation driven both thermally and by pressure, and in particular by analysis of long time...n...reorganization into the amorphous state, thereby explaining both the formation and semiconducting character of the amorphous phases. Our understanding of the process is based on phase transformation driven both thermally and by pressure, and in particular by analysis of long time...n...amorphization process. We demonstrate the equivalence of thermal and pressure-driven interconversions in a system where vacancies are either at very low levels or entirely absent. These discoveries open a new pressure-driven phase interconversion pathway.

4:42PM X21.00012 Structural, optical, and thermal stability properties of CdZnO thin films grown by molecular-beam epitaxy (MBE)1. ZHENG YANG, LIN LI, SHENG CHU, JIEYING KONG, JIALIN LIU, Quantum Structures of Laboratory, Department of Electrical Engineering, University of California, Riverside, California 92521 — CdZnO thin films with near-band-edge emission from violet (3.07 eV) to orange (2.04 eV) were grown using MBE. The CdZnO thin films evolve from pure wurzite (wz) structure to mixture of wz and rocksalt (rs) structures, and finally to pure rs structure, with increasing Cd concentration. Wz CdZnO shows a robust thermal stability than the rs CdZnO. The temperature dependence of the CdZnO bandgap shrinkage was investigated and analyzed based on the empirical Varshni and Bose-Einstein fitting of the...n...amorphization process. We demonstrate the equivalence of thermal and pressure-driven interconversions in a system where vacancies are either at very low levels or entirely absent. These discoveries open a new pressure-driven phase interconversion pathway.

4:54PM X21.00013 Electronic properties and stabilities of bulk, nano-cluster, and low-index surfaces of SnO in comparison with SnO2: application to high-temperature gas sensor. YUHUA DUAN, National Energy Technology Lab — High-temperature gas sensors to detect various components of the gas flow in gasification technologies are highly desired. As one kind of the wide band-gap oxide semiconductors, tin oxides (SnO2, SnO) are widely used as solid state sensor material, oxidation catalyst and transparent conductor. Due to the electronic structure and possibility of two different oxidation states of Sn1+ and Sn2+ and high thermal stability, tin oxides are very sensitive to oxidizing and reducing many kinds of gases, and therefore can be used to detect these gases with good sensitivity at high-temperature. In this study, based on density functional theory approach with an empirical correction of van der Waals interactions, the structural and electronic properties of the bulk, nano-cluster, and low-index surfaces of SnO2 and SnO are obtained. Our results indicate that the differences between SnO2 and SnO are significant and the controllable type of SnO2 nano-clusters have a great application in high-temperature sensor technology. In SnO, the van der Waals interactions play an important role and rule may lead to more active sites for interacting with other molecules. By investigating the interactions between gas molecules (such as CO2, H2O, C2H5, etc.) with the surfaces of SnO2 and SnO, the sensing mechanism of tin oxides will be explored.

5:06PM X21.00014 UV Induced Room Temperature Persistent Photocurrent in In2O3 Films. RAGHAVAN PANGULURI, A. DIXIT, C. SUDAKAR, P. KHAREL, PUSHKAL THAPA, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201, I.A. AVRUTSKY, Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI 48201, ALEXANDER EFROS, Center for Computational Materials Science, Naval Research Laboratory, Washington DC 20375, R. NAIK, G. LAWES, B. NADGORNY, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201. We have investigated the effects of UV irradiation on the electrical and optical properties of In2O3 thin films. These films were grown on sapphire substrate by RF sputtering. Hall effect measurements carried out to measure the carrier concentrations, n, show n-type conduction, with n = 2 x 1016 cm−3. We find that UV illumination on In2O3 films leads to a dramatic increase in the charge carrier concentration, approximately one order of magnitude, and that these elevated carrier densities persist at room temperature on a timescale of days. Consequently, we observe distinct changes in the optical absorption spectra. Also, we studied the decay of the charge carrier density to the pre-illuminated state as a function of temperature. We will discuss possible mechanisms for persistent photocconductivity in these In2O3 thin films.
and devices, but more recently has been the subject of study as a rare-earth host. It is believed that Gd$_2$O$_3$ makes a good host for these dopants due to the similarity in ionic radii between the gadolinium ion and the rare-earth dopants. The reported long radiative lifetimes of rare earth dopants in this material make it interesting for optically pumped laser materials. In this study, europium-doped gadolinium oxide (Eu$_2$Gd$_2$O$_7$) polycrystalline thin films were deposited on sapphire substrates by pulsed laser deposition at 5 and 50 mTorr oxygen pressure. Changes in the crystal structure were observed by x-ray diffraction and photoluminescence. Low-temperature photoluminescence spectra of the $^5$D$_0-^7$F$_J$ transitions in the europium ion were recorded with high resolution. Because the $^5$D$_0-^7$F$_2$ transition in europium is not subject to fine structure splitting, it provides a useful mechanism for investigation of the local environment. The $^5$D$_0-^7$F$_2$ transition is of interest as it results in the most intense emission, making europium doped material useful for red light-emitting phosphors. Radiative lifetimes of the observed transitions are also reported.

Thursday, March 19, 2009 2:30PM - 5:30PM – Session X22 GMAG DMP FIAP: Focus Session: Magnetism in II-VI and IV Semiconductors

2:30PM X22.00001 Magnetization studies of II-VI semiconductor columnar quantum dots with type-II band alignment

1 Supported in part by CSEQuIN and the Office of the Provost at UB

2:42PM X22.00002 Transition metal-doped Sb$_2$Te$_3$ magnetic semiconductor thin films

1 CHANG-PENG LI, YI-JIUNN CHIEN, LYNN DAVIES ENDICOTT, CTRAD UHER, Physics Dept., Univ. Michigan — With the doping of vanadium in tetradymite-based Sb$_2$Te$_3$, magnetic semiconductor thin films Sb$_{2-x}$V$_x$Te$_3$ have been prepared on (0001) sapphire substrates by low-temperature molecular beam epitaxy. X-ray diffraction measurements and RHEED patterns confirm single-crystalline films growing along the c-axis direction. Magnetic and anomalous Hall measurements clearly show strong ferromagnetic ordering with the easy axis along c-axis direction up to Curie temperature, which increases nearly linearly with the content of V incorporated in the lattice. So far, a high Curie temperature of 213 K has been achieved for the composition of Sb$_{1.55}$V$_{0.45}$Te$_3$.

3 This work is supported by National Science Foundation Grants

2:54PM X22.00003 MCD investigation on Mn doped CdSe Quantum Ribbons

KRITSANU TIVAKO-RAISATHORN, XINYU LIU, MARGARET DOBROWSOLKA, JACEK K. FURDYNA, University of Notre Dame, JUNG H. YU, JIN JOO, DONG W. LEE, JAE S. SON, TAEHWAN HYEON, JIWON PARK, YOUNG-WOON KIM, Seoul National University — We have successfully incorporated manganese ions into CdSe quantum ribbons with a thickness of 1.4 nm. The magnetic exchange interactions between the Mn ions are indeed present in the CdSe nanoribbons with Mn concentration ranging from 0.7 to 6.4%. The magnetic circular dichroism (MCD) spectra of Mn-doped CdSe quantum ribbons show that the Mn ions are indeed present in the CdSe nanoribbons.

3:06PM X22.00004 Fine Structure of PbSe Colloidal Nanostructures

J. G. TISCHLER, T. A. KENNEDY, E. R. GLASER, E. E. FOOS, T. J. ZEGA, R. M. STROUD, A. L. EFROS, S. C. ERWIN — Although much work has been done on PbSe nanocrystals in order to understand excited states, little is known of the ground state fine structure. Bulk PbSe is a semiconductor material with a direct band gap at the L point. The band structure at this symmetry point is four-fold degenerate for both electrons and light holes, and conduction and valence bands possess similar effective masses and g-factors. In this work, we synthesized high quality PbSe nanocrystals and characterized them using transmission electron microscopy and photoluminescence. Low-temperature photoluminescence spectra of the $^2$D$_0-^2$F$_J$ transitions in PbSe were recorded with high resolution. Because the $^2$D$_0-^2$F$_2$ transition is not subject to fine structure splitting, it provides a useful mechanism for investigation of the local environment. The $^2$D$_0-^2$F$_2$ transition is of interest as it results in the most intense emission, making PbSe doped material useful for red light-emitting phosphors. Radiative lifetimes of the observed transitions are also reported.

3:18PM X22.00005 Tunable magnetic exchange interactions in manganese-doped inverted core-shell ZnSe-CdSe nanocrystals

1 DAVID BUSSIAN, SCOTT CROOKER, MING YIN, Los Alamos National Lab, MARCIN BRYNDA, University of California-Davis, ALEXANDER EFROS, Naval Research Lab, VICTOR KLIMOVA, Los Alamos National Lab — Magnetic doping of semiconductor nanocrystals is pursued for applications in paramagnetic memory and spin-based electronics. A primary goal is to control interactions between carriers (electrons and holes) and the embedded magnetic atoms. We have demonstrated a tunable magnetic sp-d exchange interaction between electron-hole excitations and paramagnetic Mn$^{3+}$ ions using ‘inverted’ core-shell nanocrystals composed of Mn$^{3+}$-doped ZnSe cores overcoated with undoped shells of narrower-gap CdSe. Magnetic circular dichroism studies reveal giant Zeeman spin splittings of the band-edge exciton that are tunable in magnitude and sign. Effective exciton g-factors are controllably tuned from -200 to +30 at 1.6 K by increasing the CdSe shell thickness, demonstrating that strong quantum confinement and wavefunction engineering in heterostructured nanocrystals can be utilized to manipulate carrier-Mn$^{3+}$ wavefunction overlaps and the sp-d exchange parameters themselves. *D. Bussian et al., Nature Materials, in press.

1 Supported in part by the Chemical Sciences, Biosciences, and Geosciences Division of the Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy (DOE), the DOE Center for Integrated Nanotechnologies, and Los Alamos LDRD funds.
3:30PM X22.00006 Observation of Exchange Enhanced Zeeman Splitting in (Zn,Mn)Se Nanowires. B. J. COOLEY, T. CLARK, B. LIU, C. EICHFELD, E. DICKEY, S. MOHNEY, N. SAMARTH, Materials Research Institute, Penn State University, S. A. CROOKER, National High Magnetic Field Lab, Los Alamos, C. E. PRYOR, M. E. FLATTE, Dept. of Physics, University of Iowa. — Magnetic semiconductor nanowires (NWs) are of potential interest as model systems for studying the physics of spin polarized 1D Fermi liquids. A high degree of spin polarization is anticipated from the spin-d exchange-enhanced Zeeman splitting of band edge states. Here, we report the vapor-liquid-solid growth of Mn-doped amorphous Si andGe matrices, in great contrast to the previous speculation that these two should behave very similar as the semiconductor host for transition metals. While we observed a large local moment of Mn in a-Ge, Mn moment is quenched in a-Si. The large difference of local magnetic moment of Mn in a-Si and a-Ge can be understood by the local atomic environment at the magnetic dopant sites, that is, the bond length and the coordination. Statistical DFT calculations shows that the magnetic dopant Mn with less coordination and large bond length hold large magnetic moment. Otherwise, the magnetic moment would be killed. In a-Ge, dopant Mn favours less coordination and large bond while more coordination and small bond length in a-Si, which result in the enhancement/quenchment of local magnetic moment Mn in a-Si/a-Ge.

The work is supported by DOE (Grant No. DEFG02-05ER46237). Calculations were performed on computers at NERSC.

4:06PM X22.00009 Magnetism of Mn doped in a-Si and a-Ge 1. JUEXIAN CAO — With experimental studies and density function theory calculations, we report on the properties of Mn-doped amorphous Si and Ge which are designed to understand the fundamentals of cooperative phenomena in highly correlated electronic and magnetic systems. We observed a striking difference in Mn local moment when doped in a-Si and a-Ge matrices, in great contrast to the previous speculation that these two should behave very similar as the semiconductor host for transition metals. While we observed a large local moment of Mn in a-Ge, Mn moment is quenched in a-Si. The large difference of local magnetic moment of Mn in a-Si and a-Ge can be understood by the local atomic environment at the magnetic dopant sites, that is, the bond length and the coordination. Statistical DFT calculations shows that the magnetic dopant Mn with less coordination and large bond length hold large magnetic moment. Otherwise, the magnetic moment would be killed. In a-Ge, dopant Mn favours less coordination and large bond while more coordination and small bond length in a-Si, which result in the enhancement/quenchment of local magnetic moment Mn in a-Si/a-Ge.

1Supported by US DOE (Grant No. DEFG02-05ER46237). Calculations were performed on computers at NERSC.

3:54PM X22.00008 Effects of defects on the half metallicity of a Mn/Si digital ferromagnetic heterostructure. MICHAEL SHAUGHNESSY, RYAN SNOW, CHING FONG, UC Davis — The effects of defects on the half-metallic properties of the Mn/Si digital ferromagnetic heterostructure (DFH) (PRL 96, 027211 (2006)) are investigated using a first principles density-functional theory approach. The half metallicity is retained when the Mn layer is recovered in quantum wells, in which the thickness of the Mn layer would be smaller than the region visited by the holes. [1] H. Boukari et al., Phys. Rev. Lett. 88, 207204 (2002); [2] D. Kechrakos et al., ibid 94, 127201 (2005).

4:30PM X22.00011 Ferromagnetic ordering of Mn-As co-doped Ge as diluted magnetic semiconductors studied within a Heisenberg model 1. HUA CHEN, U of Tennessee-Knoxville, WENGLUAN ZHU, ZHENYU ZHANG, U of Tennessee-Knoxville;Oak Ridge National Laboratory — To achieve room temperature ferromagnetism in group-IV-based diluted magnetic semiconductors, it is required to increase the concentration of magnetic dopant Mn in the host semiconductors. A recent theoretical study has suggested that the concentration of substitutional Mn in Ge can be greatly enhanced upon co-doping with As, an n-type electronic dopant [1]. Using Monte Carlo simulations based on a classical Heisenberg model with the magnetic coupling parameters calculated from first principles, we study the magnetic property of Mn and As co-doped Ge at low doping concentrations. The estimated Curie temperature increases almost linearly with increasing Mn doping concentration and reaches 264K at 5% Mn. In contrast, at the same doping level pure Mn doped Ge does not show any finite temperature ferromagnetic ordering. [1] W. G. Zhu, Z. Y. Zhang, and E. Kaxiras, Phys. Rev. Lett. 100, 027205 (2008).

1Supported by DMSE/BES of USDOE and USNSF.
The low temperature thermopower of the 2DES at the 2D system at $\nu$ schemes for detecting this degeneracy rely on interferometric braiding operations, it may also have thermodynamic implications. In particular, the entropy of the non-abelian Moore-Read paired composite fermion state. A key attribute of this state is its large degeneracy when quasiparticles are present. While most

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The essence of the $\nu = 5/2$ fractional quantum Hall effect is believed to be well captured by the Moore-Read Pfaffian (or anti-Pfaffian) description. However, an important mystery regarding the formation of the Pfaffian state is the role of the three-body interaction Hamiltonian $H_3$ that produces the Pfaffian as an exact ground state and the concomitant particle-hole symmetry breaking. We show that a two-body interaction Hamiltonian $H_2$ constructed via particle-hole symmetrization of $H_3$ produces a ground state nearly exactly approximating the Pfaffian and anti-Pfaffian states, respectively, in the spherical geometry. More importantly, the ground state energy of $H_2$ is shown to exhibit a `Mexican-hat' structure as a function of particle number in the vicinity of half filling for a given flux indicating spontaneous particle-hole symmetry breaking.

3:18PM X23.00005 Jack Polynomials, W-algebras and application to Fractional Quantum Hall Effect

STEVEN H. SIMON, Oxford University, B. ANDREI BERNEVIG, Princeton University, VICTOR GURARIE, University of Colorado — We examine Jack symmetric functions and certain W-algebras as schemes for generating fractional quantum Hall wavefunctions. We add substantially to the evidence that the Ising anyons correspond to certain W-algebras, by calculating the central charge and scaling dimensions of some of the fields in both cases and showing that they match. Except for the Read-Rezayi series all of these Jack symmetric functions turn out to be nonunitary theories. We discuss the (perhaps optimistic) possibility that these approaches may have relevance to various physical quantum Hall systems. Open questions in the field, as well as why this is of importance to those concerned with real experiments, will also be discussed.

3:30PM X23.00006 Resources needed for performing Shor’s algorithm with Ising Anyons

MARA BARABAN, Yale University, STEVEN SIMON, Oxford University, NICK BONESTEEL, Florida State University — While Ising anyons, the presumed quasi-particles of the $\nu = 5/2$ fractional quantum Hall state, do obey non-Abelian statistics, their braid group is not sufficiently rich to support universal quantum computation (UQC). Recently, Bravyi [1] proposed a method for combining topological and non-topological operations that exploits the topological protection of the Ising anyons to allow for UQC even with very low accuracy non-topological operations. Starting from Bravyi’s proposal, we calculate the resources required to perform Shor’s algorithm. We find that when parallelization is included, the required number of qubits grows as the number of gates ($\sim N^3$, where $N$ is the length of the number to be factored using Shor’s algorithm) and that the total time required is nearly independent of $N$. Numerical work has further allowed us to determine how far apart the anyons must be in a realistic sample in order to perform topological operations. We thus estimate how large a coherent sample would be required for Ising anyons to successfully execute modular exponentiation. We compare our results to the requirements for performing Shor’s algorithm via fully topological quantum computation with Fibonacci anyons, the presumed quasiparticle excitation of the $\nu = 12/5$ fractional quantum Hall state. [1] S. Bravyi, Phys. Rev. A 73, 042313 (2006)
4:30PM X23.00011 Probing the neutral edge modes in transport across a point contact via thermal effects in the Read-Rezayi non-abelian quantum Hall states, EYTAN GROSFELD, University of Illinois, SOURIN DAS, Center for High Energy Physics, Indian Institute of Science, Bangalore, India — Non-abelian quantum Hall states are characterized by the existence of neutral gapless edge modes, whose structure is intricately related to the existence of bulk quasi-particle excitations obeying non-abelian statistics. Detecting the presence of these neutral modes is thus an important step towards establishing the non-abelian nature of these quantum Hall states. While it is hard to couple to the neutral modes using an electric field, they will directly couple to a temperature gradient and respond by contributing to the thermal current. By obtaining an expression for the thermal current through a quantum point contact, we demonstrate that a measurement of the thermal current will reveal the presence of the neutral modes. In addition, since thermal measurements are difficult to implement, we propose a setup which uses no external heaters and relies solely on noise measurements to detect thermal effects. The idea is to have two point contacts in series separated by a distance set by the thermal equilibration length of the charge mode. We show that by using the first point contact as a heating device, the excess charge noise measured at the second point contact carries a non-trivial signature of the presence of the neutral mode hence leading to its indirect detection.

4:42PM X23.00012 Charge-statistics separation and probing non-Abelian states for quantum Hall plateau at $\nu=5/2^*$, FEIFEI LI, DIMA FELDMAN, Department of Physics, Brown University, Providence, Rhode Island 02912, USA — Several states were proposed for quantum Hall plateau at $\nu=5/2$. We suggest a transport experiment that can distinguish six of the candidate states. The proposal involves measurements of current and shot noise in a geometry with three quantum point contacts. Unlike interference experiments, this approach can distinguish Pfaffian and anti-Pfaffian states as well as different states with identical Pfaffian or anti-Pfaffian statistics. Moreover, the transport is not sensitive to the fluctuations of the number of quasiparticles trapped in the system. [1] D. E. Feldman and Feifei Li, Phys. Rev. B 78, 161304(R) (2008).

4:54PM X23.00013 Quantum Hall hierarchy revisited, SUSANNE VIEFERS, JUHA SUORSA, University of Oslo, HANS HANSSON, MARIA HERMANNS, Stockholm University — Using techniques from conformal field theory, we construct explicit candidate wave functions for the entire Abelian quantum Hall hierarchy, i.e. quasihole- and quasielectron condensates, as well as mixtures of these. The formalism presented here, generalizes and unifies our previous techniques, which were only able to address quasielectron condensates. In the special cases of the positive and negative Jain sequences $\nu = n/(2np \pm 1)$, our method exactly reproduces Jain’s composite fermion wave functions. In general our results are consistent with Wen’s topological classification of FQH states.

5:06PM X23.00014 Non-Abelian quasielectrons, HANS HANSSON, MARIA HERMANNS, Stockholm University, SUSANNE VIEFERS, University of Oslo — Using methods from conformal field theory, we construct trial wave functions for quasielectron excitations in both Abelian and non-Abelian quantum Hall states. We briefly explain the underlying theory, and present analytical and numerical results for the case of two and four quasielectrons in the non-Abelian Moore-Read pfaffian state. Our methods generalize to other non-Abelian states, and can possibly also give a description of condensates of non-Abelian quasielectrons.

5:18PM X23.00015 Topological Entanglement Entropy of Realistic Quantum Hall States, BARRY FRIEDMAN, Department of Physics, Sam Houston State University, GREG LEVINE, Department of Physics and Astronomy, Hofstra University — The entanglement entropy for the incompressible states of a realistic quantum Hall system was studied by direct diagonalization for square clusters with periodic boundary conditions. The subdominant term to the area law, the topological entanglement entropy, was extracted for filling factors 1/3 and 5/2. The result for filling factor 1/3 is consistent with the topological entanglement entropy for the Laughlin wave function while the 5/2 filling factor exhibits a topological entanglement entropy consistent with the Moore-Read wave function. Preliminary results for the topological entanglement entropy for other incompressible states in the second Landau level will be discussed.


2:30PM X24.00001 "Developments in the application of borohydrides for hydrogen storage". ERIC MAUZOU, U of Missouri — No abstract available.

3:06PM X24.00002 First-Principles Determination of Crystal Structures, Phase Stability, and Reaction Thermodynamics in the Li-Mg-Al-H Hydrogen Storage System1, ALIREZA AKBARZADEH2, California State University Northridge, CHRIS WOLVERTON3, Northwestern University, VIDVUDS OZOLINS4, University of California Los Angeles — First-principles DFT calculations have been used to investigate the crystal structures, thermodynamic stability, and decomposition pathways of Li-Mg-Al-H hydrogen storage compounds. We find that the recently discovered LiMg(AlH4)3 compound is marginally stable with respect to decomposition into LiAlH4 and Mg(AlH4)2; however, we also find that LiMg(AlH4)3 is unstable with respect to H2 release and decomposes exothermically into LiMgAlH4, Al, and H2 in excellent agreement with measurements. Using ICSD crystal structures database, we predict that the hypothetical MgAlH4 compound should assume the orthorhombic BaGaF2 prototype structure. We also discuss that phonon vibrations have sizeable effects on the enthalpies and entropies of hydrogen release reactions of Li-Mg-Al-H compounds.

1This research was supported by the US Department of Energy under grant DE-FG02-05ER46253
2Dept. of Physics & Astronomy
3Dept. of Materials Science and Engineering
4Dept. of Materials Science and Engineering
ACATRINEI, SAURABH KABRA, LUKE DAEMEN, LANCE-LEC, LANL, Los Alamos, NM 87545, USA — CuMg stoichiometry. NiMg$_2$x of formation of the hydride is related to that of the primary alloy, it was hypothesized that CuLi to the properties of the hydrogenated (and deuterated) CuLi$_2$NiMg−reason, much effort has been put toward lowering their thermal stability. One of the common routes taken to achieve this aim is to mix with other borohydrides to the Li-doped CuMg metal borohydrides, soft modes in LTI and in Mg-substituted CaMgNiH$_2$, are available in the published literature. We calculate the enthalpy of formation ∆H with density functional theory (DFT) for both using three different approximations for the exchange-correlation energy functional. Phonon spectra are calculated as well. DFT unequivocally identifies LTII as preferable since ∆H obtained for it is in better agreement with experiment and its phonon spectrum contains no anomalies. Structures approximating LTII derived from analyses of soft modes in LTI and in Mg-substituted CaMgNiH$_2$ are also discussed.

Mg$_2$NiH$_4$, JAN HERBST, LOUIS HECTOR, JR., GM R&D Center — Mg$_2$NiH$_4$ is a semiconductor and forms an ordered low temperature monoclinic phase and a disordered high temperature cubic modification. Two distinct structures for the monoclinic phase from neutron diffraction studies of the deuterated analog, which we designate as LTI and LTII, are present in the published literature. We calculate the enthalpy of formation ΔH with density functional theory (DFT) for both using three different approximations for the exchange-correlation energy functional. Phonon spectra are calculated as well. DFT unequivocally identifies LTII as preferable since ΔH obtained for it is in better agreement with experiment and its phonon spectrum contains no anomalies. Structures approximating LTII derived from analyses of soft modes in LTI and in Mg-substituted CaMgNiH$_2$ are also discussed.

Hydrogen Storage in Cu-Li-Mg Alloys, M. HELENA BRAGA$^2$, GEORGE CHERTKOV, ALICE Acatrinei, Saurabh Kabra, Luke Daemen, Lance-Lc, Lanl, Los Alamos, NM 87545, USA — CuMg does not form a hydride. However CuLi$_2$Mg$_2$−$_2$ (x ~ 0.11) has a hexagonal crystal structure (P6$_3$22), just like NiMg$_2$, a compound known for its hydrogen storage properties. A comparison between the phase diagrams of the systems Cu-Mg and Ni-Mg shows that these binary systems form compounds with similar stoichiometry. NiMg$_2$ is formed by peritectic reaction of the elements at 759 °C (1032 K) and CuMg$_2$ at 508 °C (841 K) by congruent melting. Since the energy of formation of the hydride is related to that of the primary alloy, it was hypothesized that CuLi$_2$Mg$_2$−$_2$...
4:42PM X24.00010 Hydrogen Desorption Behavior of Nickel-Chloride-Catalyzed Stoichiometric \text{Li,BN}_3\text{H}_{10}, FREDERICK PINKERTON, MARTIN MEYER, General Motors R&D Center — Li-B-N-H quaternary hydrides with the \(\alpha\)-phase crystal structure form over a range of compositions between Li\(_2\)BN\(_3\)H\(_4\) and Li\(_2\)BN\(_3\)H\(_{10}\) and have up to 11.9 wt\% hydrogen capacity. Previous work focused on the non-equilibrium Li\(_2\)BN\(_3\)H\(_4\) composition created by ball milling because it has maximum hydrogen release and minimum NH\(_3\) co-generation. Here we report the hydrogen and NH\(_3\) release characteristics of \(\alpha\)-phase material having the equilibrium Li\(_2\)BN\(_3\)H\(_{10}\) composition. In the absence of a dehydrogenation catalyst, H\(_2\) and NH\(_3\) were released simultaneously in roughly equal quantities by weight (or about 10\% NH\(_3\) by volume) at temperatures above 240 \(^\circ\)C. Adding Ni in the form of NiCl\(_2\) as a dehydrogenation catalyst reduced the H\(_2\) release temperature by 122 \(^\circ\)C. NH\(_3\) release, in contrast, still occurred only at the higher temperature. As a result, decomposition occurred in two steps separated in temperature, dominated by H\(_2\) gas at low temperature and NH\(_3\) at high temperature. The two gases clearly evolved in two distinct reactions that are coincident in uncatalyzed Li\(_2\)BN\(_3\)H\(_{10}\), but can be separated by a dehydrogenation catalyst. We expect that NH\(_3\) co-generation could be completely eliminated at sufficiently low dehydrogenation temperatures.

4:54PM X24.00011 Thermochemical Investigations of Nano-phase Ammonia Borane: Effect of Higher Loading, ABHI KARKAMKAR, Pacific Northwest National Laboratory, ASHLEY STOWE, TOM AUTREY — Chemical hydrogen storage materials that release H\(_2\) by thermolysis without generating CO\(_2\) offer an attractive option. The ammonia borane is an attractive compound containing more than 18 wt\% hydrogen. However, the kinetics of hydrogen release in not favorable in bulk materials where H\(_2\) is released at 114 \(^\circ\)C. We recently reported use of SBA-15 as scaffold material to form a nanophase ammonia borane species which liberated H\(_2\) at significantly lower temperatures. Hydrogen formation from bulk AB is slightly exothermic (-5 kcal/mol). The reaction enthalpy (\(\Delta H\)) for release of H\(_2\) from AB adsorbed into SBA-15 (1:1 w/w) was determined to be nearly thermoneutral—dramatically lower than the bulk material. Near thermoneutral reaction suggests that there would be less restrictive heat management issues, greater thermal stability and potentially a lower energy input requirement for regeneration of AB. One drawback which results for nano-phase AB is that while the hydrogen release properties are enhanced, the gravimetric hydrogen density is reduced by a 50\% for the 1 to 1 by mass ratio material. We here report on our efforts to increase the gravimetric hydrogen density of nano-phase AB by developing higher loading conditions of AB adsorbed into mesoporous silica (MCM-41).

5:06PM X24.00012 Hydrogen storage in ammonia borane: \textit{Ab initio} study of the de- and rehydrogenation mechanisms, KISEOK CHANG, DAVID TOMANEK, Michigan State University, EUNJU KIM, PHILIPPE F. WECK, University of Nevada Las Vegas — Using \textit{ab initio} density functional calculations, we study the microscopic mechanism of hydrogen release from ammonia borane (NH\(_3\)BH\(_3\)) and the reverse process leading to its subsequent recharging with hydrogen. Our total energy surfaces indicate the most favorable pathways to thermally convert the NH\(_3\)BH\(_3\) molecular solid to the energetically preferred polymer NH\(_3\)BH\(_2\) and molecular hydrogen. To prevent formation of undesirable side-products such as the cyclic compound borazine (N\(_3\)B\(_3\)H\(_6\)) or other complexes that would prevent subsequent rehydrogenation, we propose to enclose AB in narrow carbon nanotubes. In this constrained space, we investigate possible rehydrogenation pathways using atomic and molecular hydrogen as well as selected protonation agents.

\(1\)Supported by NSF NSEC Grant 425826 and NSF-NIRT grant ECS-0506309.

\textbf{Thursday, March 19, 2009 2:30PM - 5:42PM — Session X25 DMP: Focus Session: Graphene XVII: p-n Junctions, Nanoribbons, and Quantum Dots 327}

2:30PM X24.00021 Theoretical investigations of deformed graphene nanoribbons, RICARDO KAGIMURA, MARIO S. C. MAZZONI, HELIO CHACHAM, Universidade Federal de Minas Gerais — Graphene nanoribbons (GNRs) have attracted considerable attention in the last two years. Recent experimental work [Science, 319, 1229 (2008)] has reported semiconducting GNRs with width of a few nanometers and suitable band gaps for electronic applications. One desirable aim in the investigation of GNRs is to control their electronic properties. It has been proposed, for instance, that chemical edge modifications or external strain can modify their electronic properties. In this work, we report density functional calculations, we study the microscopic mechanism of hydrogen release from ammonia borane (NH\(_3\)BH\(_3\)) and the reverse process leading to its subsequent recharging with hydrogen. Our total energy surfaces indicate the most favorable pathways to thermally convert the NH\(_3\)BH\(_3\) molecular solid to the energetically preferred polymer NH\(_3\)BH\(_2\) and molecular hydrogen. To prevent formation of undesirable side-products such as the cyclic compound borazine (N\(_3\)B\(_3\)H\(_6\)) or other complexes that would prevent subsequent rehydrogenation, we propose to enclose AB in narrow carbon nanotubes. In this constrained space, we investigate possible rehydrogenation pathways using atomic and molecular hydrogen as well as selected protonation agents.

\(2\)This work was supported by the Brazilian agencies - CNPq and CAPES.

2:42PM X25.00002 Quantum Dot Behavior in Graphene Nanoconstrictions, KATHRYN TODD, HUNG-TAO CHOU, SAMI AMASHA, PATRICK GALLAGHER, DAVID GOLDBABER-GORDON, Stanford University — Graphene nanoribbons have been proposed as novel high-frequency transistors due to their high mobility and transport gap that scales inversely with width. In order to understand the origin of the transport gap in long nanoribbons, we measure transport through short side-gated nanoconstrictions. Unlike in long (\(\geq 250\) nm) nanoribbons, we measure transport through multiple quantum dots in series, shorter (\(\leq 60\) nm) constrictions display behavior characteristic of single and double quantum dots. We find that dot size scales with constrictions width. In the narrowest short constrictions, high on/off ratios are achievable, while in wider (\(\geq 35\) nm) constrictions we observe quantum dot behavior overlaid on a highly conducting background. We hypothesize that the metal side gates in close proximity to our short constrictions suppress the importance of edge disorder, and compare constrictions fabricated with and without metal side gates. We propose a model where transport occurs through quantum dots nucleated by disordered background potential in the presence of a confinement gap.

2:54PM X25.00003 Interaction effects in graphene p-n junctions, LINGFENG MATTHEW ZHANG, University of California, San Diego — We review our recent analytical and numerical studies of a new class of graphene devices: lateral p-n junctions. Such structures are realized experimentally by modulating the electron density in graphene samples with external gates. Our theory describes the charge density distribution, the electric field profile, and the resistance of such p-n junctions. The proper treatment of the electrostatic screening beyond the linear order is crucial for obtaining correct results for all these quantities. In particular, the electric field at the interface of the electron and hole regions is strongly enhanced due to limited screening capacity of Dirac vacuum. This nonlinear screening effect can significantly reduce the junction resistance. It is necessary to include it in order to obtain a good agreement with the experiments. More subtle interaction effects such as the Bragg reflection of quasiparticles on Friedel oscillations near the p-n interface are also discussed.

\(3\)This work is done in collaboration with M. M. Fogler and is supported by the NSF and the ASC UCSD.
3:30PM X25.00004 Effect of Shape on Electronic and Magnetic Properties of Graphene Nanoribbons (GNRs) | ALBERT K. DEARDEN, PHILIP SHEMELLA, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute. Troy, NY. PULICKEL M. AJAYAN, Dept. of Mechanical Engineering & Materials Science, Rice University, Houston, TX. SARIOJ K. NAYAK, Department of Physics, Applied Physics, & Astronomy, Rensselaer Polytechnic Institute. Troy, NY. We have studied electronic and magnetic properties of graphene nanostructures with different shapes. In particular, we have studied both zigzag and armchair graphene nanoribbons (GNR) of triangular shape using density functional method. We find electronic and magnetic properties of triangular structures are drastically different from their rectangular counterparts and our results suggest that, in addition to size effect, shape of the structure has a large impact on the underlying electronic properties of GNRs. We will compare our results with available experiments.

3:42PM X25.00005 Probing the transport gap in edge disordered graphene nanoribbons | MELINDA HAN, PHILIP KIM, Columbia University. We present experimental studies on the detailed nature of the transport gap observed in etched graphene nanoribbons. Temperature dependent measurements of electronic transport in the “gapped” region of suppressed conductance suggest transport via localized states or charge islands, giving rise to separate energy scales for hopping conductance and the transport gap. Distinct temperature regimes with different exponential temperature dependences are observed, with a crossover temperature dependent on ribbon width. A transition to “bulk” graphene electronic behavior is observed for wider ribbons, and the size of the transport gap shows a length dependence consistent with conduction due to hopping.

3:54PM X25.00006 Role of edge states in graphene nano-ribbons: - DFT studies | SUMIT SAXENA, TREVOR A. TYSON, Dept. of Physics, New Jersey Institute of technology. Newark, NJ. We present first principle calculations to study the effect of edge states in graphene nano-ribbons. Spin restricted calculations for graphene nano-ribbons were performed using ground state density functional theory. The plot of electron localization function corresponding to the edge dangling bonds has revealed highly reactive edge states in graphene nano-ribbons. The reactivity of the graphene nano-ribbons with respect to the edge structure is discussed. This study has been supplemented by band structure studies in armchair and zigzag edged graphene nano-ribbon systems. This work is supported in part by NSF DMR-0512196.

4:06PM X25.00007 Electronic properties of Graphene quantum dots | PAWEL HAWRYLAK, Institute for Microstructural Sciences NRC, Ottawa, PAWEL POTASZ, Wroclaw University of Technology, Poland. We study electronic properties of Graphene quantum dots in magnetic fields. Graphene quantum dots are atomically thick nanometer-scale islands constructed by connecting benzene molecules. Quantum dots with triangular and hexagonal shape have shown to have different edge properties [1,2], and triangular zig-zag structures have recently attracted attention due to their half-filled zero-energy edge states. In this work, we investigate electronic and magnetic properties of triangular and hexagonal shaped islands. We study the effect of first and second nearest neighbour interactions, magnetic field and the number of atoms on the single-particle properties using a tight-binding model. We then use configuration interaction method to study the effect of electron-electron interactions on the ground state properties including magnetization, excitation spectra, and their effect on Coulomb blockade and tunneling through graphene islands. [1] J. Fernandez-Rossier and J.J. Palacios, Phys.Rev.Lett. 99, 177204 (2007); [2] M. Ezawa, Phys.Rev.B, 77, 155411 (2008).

4:18PM X25.00008 Charge transport in ballistic multipe probe bilayer graphene dots,1 | IGOR ROMANOVSKY, CONSTANTINE YANNOUTEAS, UZI LANDMAN, Georgia Institute of Technology. Atlanta, GA 30332. We present a numerical analysis of the transport properties of the bilayer graphene quantum dots attached to multiple leads. In the framework of the tight binding model and using the nonequilibrium Green’s function technique, we study numerically effects due to: magnetic fields, bias voltage between the layers, geometrical shape, and the arrangement of the attachments of the leads to the device. The results are compared to those obtained for similar quantum dot structures made from a graphene monolayer.1Supported by the US D.O.E. (FG05-86ER-45234)

4:30PM X25.00009 Graphene Josephson Qubit | COLIN BENJAMIN, JIANNIS K. PACHOS, School of Physics & Astronomy, University of Leeds. Leeds, UK. We propose to combine the advantages of graphene, such as easy tunability and long coherence times, with Josephson physics to manufacture qubits. These qubits can either be built around a 0 and π junction and controlled by external flux or a d-wave Josephson junction can itself be tuned via a gate voltage to create superpositions between macroscopically degenerate states. We show that ferromagnets are not required for realizing π junction in graphene, thus considerably simplifying its physical implementation. We demonstrate that one qubit gates, such as arbitrary phase rotations and the exchange gate, can be implemented easily.

4:42PM X25.00010 Quantum Transport in Graphene pnp Junctions with Contactless Top Gates | JAIRO VELASCO JR., GANG LIU, WENZHONG BAO, CHUN NING LAU, University of California at Riverside. We show that graphene offers the unique opportunity to explore relativistic physics in a condensed matter system. One such example is the phenomenon of Klein tunneling in graphene pnp junctions. By using a contactless top gate, we are able to fabricate very high quality pnp junctions, and perform electrical transport spectroscopy measurements in zero and finite magnetic fields. We observe oscillations in conductance of the pnp junction and changes in magnetoresistance. Latest experimental progress and comparison with theoretical predictions will be discussed.

4:54PM X25.00011 Systematic study of the transport gap and localization in graphene nanoribbons of varying lengths | PATRICK GALLAGHER, KATHRYN TODD, DAVID GOLDHABER-GORDON, Stanford University. Recent studies of very short graphene nanoconstrictions[1] have found that short constrictions lack the large transport gap displayed by longer nanoribbons, implying that localization behavior plays a critical role in the transport gap. We present transport measurements on graphene nanoribbons of constant width and varying length and report on gap characteristics and Coulomb blockade behavior. We discuss the relevant theoretical models and compare their predictions to our data.

5:06PM X25.00012 Signatures of classical chaos in gate-defined graphene quantum dots | JENS H. BARDAKRSON, Laboratory of Atomic and Solid State Physics, Cornell University. Ithaca, NY 14853-2501, USA. M. TITOV, School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK. We have studied electronic and magnetic properties of graphene nanostructures with different shapes. In particular, we have studied both zigzag and armchair graphene nanoribbons (GNR) of triangular shape using density functional method. We find electronic and magnetic properties of triangular structures are drastically different from their rectangular counterparts and our results suggest that, in addition to size effect, shape of the structure has a large impact on the underlying electronic properties of GNRs. We will compare our results with available experiments.
5:18PM X25.00013 Quantum Hall Effect in Two-Terminal Graphene Devices. JAMES WILLIAMS, Harvard University, DIMA ABANIN1, Massachusetts Institute of Technology, LEONARDO DICARLO2, Harvard University, LEONID LEVITOV, Massachusetts Institute of Technology, CHARLES MARCUS, Harvard University — We report on transport measurements in the quantum Hall regime of two-terminal single and bilayer graphene devices. The mixture of the longitudinal and transverse conductivities in the two-terminal geometry results in departures from the expected conductance values on the Hall plateaus and are found to be device-dependence dependent. The experimental results are compared to theory and discrepancies are discussed. Research supported in part by INDEX, an NRI Center, and by the Harvard NSEC.

1Present Address: Princeton University
2Present Address: Yale University

5:30PM X25.00014 New Computational Approach to Electron Transport in Irregular Graphene Nanostructures. DOUGLAS MASON, ERIC HELLER, Physics Dept., Harvard University, Cambridge, MA, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA — For novel graphene devices of nanoscale-to-macroscopic scale, many aspects of their transport properties are not easily understood due to difficulties in fabricating devices with regular edges. Here we develop a framework to efficiently calculate and potentially screen electronic transport properties of arbitrary nanoscale graphene device structures. A generalization of the established recursive Green’s function method is presented, providing access to arbitrary device and lead geometries with substantial computer-time savings. Using single-orbit nearest-neighbor tight-binding models and the Green’s function-landauer scattering formalism, we will explore the transmission function of irregular two-dimensional graphene-based nanostructures with arbitrary lead orientation. Prepared by LBNL under contract DE-AC02-05CH11231 and supported by the U.S. Dept. of Energy Computer Science Graduate Fellowship under grant DE-FG02-97ER25308.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X26 DCMP: Nanowire & Nanotube Synthesis and Properties 328

2:30PM X26.00001 Aligned Gallium Nitride Nanowire Growth by Chemical Beam Epitaxy Method. RYAN MUNDEN, App Phys, Yale Univ, ALEKSANDAR VACIC, ERIK CASTIGLIONE, WEIHUA GUAN, Elect Eng Yale Univ., CHRISTINE BROADBRIDGE, Physics, Southern CT State Univ, MARK REED, EE/AP Yale University — Gallium Nitride (GaN) Nanowires (NWs) have successfully been grown via a chemical beam epitaxy method. Source gases of Trimethylgallium (TMGa) and Ammonia (NH3) are impinged directly onto a hot growth substrate (∼800 °C) in high vacuum (∼1x10^-8 torr, base; ∼1x10^-5 torr, growth). A thin metal film acts as catalyst, but NWs were also grown without catalyst. By this method NWs have been grown on silicon, alumina, sapphire, and GaN-film substrates. NWs grown on GaN films grow aligned to the growth substrate, perpendicular to the c-plane GaN film surface. Wires aligned to the GaN a-planes can also be observed. NWs have been studied by SEM, TEM, and electrical characterization. NW widths are ∼2.5 micron with diameters of ∼25 nm. NWs are uniform, straight, and aligned with the substrate over large areas. However closer inspection of the NWs by TEM shows that the NWs are often polycrystalline in nature. There are distinct segments “stacked” into a nanowire leading to noticeable diameter variations on the nanoscale. Diameter modulation can be enhanced through choice of growth substrate, temperature, and pulsing of the TMGa source.

2:42PM X26.00002 Temperature Evolution of Gallium Nitride Nanowire Vapor-solid Growth Matrix. K. MCELROY, Michigan State University, B.W. JACOBS, Sandia National Laboratories, CA, T.R. BIELER, M.A. CRIMP, V.M. AYRES, Michigan State University — Recent results indicate that vapor-solid growth mechanisms can yield semiconductor nanowires with high crystallinity. In the present experiments, gallium nitride nanowire growth is initiated following formation of a microcrystalline growth matrix. A change in nanowire orientation from wurtzite (zinc-blende) directions at 850 °C and 950 °C to the wurtzite [0001] direction at 1000 °C is observed. The change in nanowire orientation is correlated with changes in the growth matrix. Investigations of the evolution of the growth matrix as a function of temperature using x-ray diffraction with orientation analysis, atomic fore microscopy, high-resolution transmission electron microscopy (HRTEM) and scanning electron microscopy (SEM) are presented.

2:54PM X26.00003 Interaction between the boron nitride nanotube and biological molecules. CHIH-KAI YANG, Chang Gung University — By calculating the interaction between boron nitride nanotubes (BNNT) and a variety of biological molecules, including amino acids and nitrogenous bases that are part of a nucleotide, using density functional theory, we conclude that there is no bonding or chemical adsorption between the wide band-gap BNNT and the biological molecules considered. This weak interaction suggests that BNNTs may be used as a safe nanoscale channel for transporting biological molecules.

3:06PM X26.00004 Formation of Silicon Carbide Y Junctions by the Coalescence of Catalysts. ZHENYU LIU, JUDITH C. YANG, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, 15261 PA, USA; V. SROT, PETER A. VAN AKEN, M. RÜHLE, Max-Planck-Institute for Materials Research, Heisenbergstrasse 3, D-70569, Germany — We previously reported the formation of crystalline SiC nanocones by the released ion catalytic procedure, where the initially carbon-encapsulated iron nanoparticles escape from their carbon shells and agglomerate while catalyzing 1D SiC growth. Here we show that the coalescence of the iron nanoparticles can lead to Y junctions. Y junctions where the SiC branches are either parallel or inclined with respect to each other have been observed by scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). The microstructure of the resulting products is analyzed by various techniques, including X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDS) as well as electron energy loss spectroscopy (EELS). The Y junction with two parallel branches of various diameters suggests that the Y junction can be induced by the growth kinetics attributed to the diameter dependence, such as by the Gibbs-Thomson or surface tension effect. The proposed formation mechanism of Y junctions by the coalescence of catalyst droplets is a promising method to the construction of heterostructure nanowire devices.

3:18PM X26.00005 Quantum Confinement in PbS nanowire. SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University, Houghton, MI 49931 — One dimensional nanowires have become leading candidates in building nano sensor, nano transistor, optoelectronic devices and logic circuit. In the last several years, PbS nanowire has drawn considerable interest for its potential applications in optical switch and solar cell. Controlled synthesis of PbS nanowire with diameter ranging from 1.2 nm to 20 nm have been reported with the photo luminescence study revealing wide band gap behavior for the nanowire. This offers exciting opportunities to study theoretically quantum confinement effect in PbS Nanowire. We report first principles density functional calculations of the electronic properties of PbS nanowire as a function of diameter. Our calculation shows, by varying the diameter of the nanowire from ∼1.17 nm to ∼3.64 nm, the energy band gap is found to change from 1.55 eV to 0.93 eV, substantially higher than the band gap observed for the PbS bulk confirming the role of quantum confinement.
3:30PM X26.00006 Toward complex nanostructures: lead chalcogenide nanoparticles, nanowires, and more 1, WEON-KYU KOH1, DAVID K. KIM2, CHERIE R. KAGAN3, CHRISTOPHER B. MURRAY4. University of Pennsylvania — Lead chalcogenides have been shown to be interesting semiconductor materials due to their small bandgaps and large Bohr radii. Based on lead chalcogenide nanoparticles as building blocks, we studied anisotropic growth of their nanowires and other structures. Growth mechanism of those structures is believed to oriented attachment which is mainly driven by dipole moment; in addition the role of surfactant is also important due to their dynamic binding on the nanoparticle surface. As-synthesized nanoparticles and nanowires were characterized using electron microscopy, X-ray diffraction, optical and electrical measurement. Our initial results open up new opportunities for photovoltaic device, sensor, and other application using those unique structures.

1Department of Chemistry
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3:42PM X26.00007 Optimal Annealing Conditions, Mechanism, and Applications for the Crystallization of Titania Nanotubes Powders Obtained by Anodization, EUGEN PANAITESCU, LATIKA MENON, Northeastern University, Physics Department — Titanium oxide nanotubes have drawn recent interest due to their possible application in photocatalysis, water splitting and photovoltaics, as they combine the wide gap semiconductor properties of the material with the high surface per unit volume of the nanostructures. Amorphous ordered titania nanotubes arrays can be obtained by anodization of titanium foils, and our group developed a method of ultrafast synthesis of powders containing such nanotubes bundles. Crystallization can be achieved by annealing, and we investigated the influence of annealing parameters using differential scanning calorimetry coupled with spectroscopy and imaging techniques such as SEM, TEM and XRD. Our extensive study revealed the optimal parameters for crystallization without structural damage at the nanoscale, which can occur for temperatures as low as 270 degrees Celsius. Mechanistic explanations and numerical studies offered us a theoretical insight on the phase transition process. Further employing of our crystalline powders in dye sensitized solar cells revealed efficiency results superior to those previously reported for crystallization at higher temperatures and annealing rates.

3:54PM X26.00008 Controlled Attachment of Gold Nanoparticles on Ordered Titania Nanotube Arrays. MOHAMED ABDIELMOULA, EUGEN PANAITESCU, Physics Department, Northeastern University, CHRISTIAAN RICHTER, Yale University, LAURA LEWIS, Department of Chemical Engineering, Northeastern University, LATIKA MENON, Physics Department, Northeastern University — Gold nanoparticles have been deposited on electrochemically synthesized high-aspect ratio Titania nanotubes. Titania nanotubes with very long aspect ratio as long as 50microns are synthesized by means of electrochemical anodization of titanium foils in chlorine containing electrolytes. The tube dimensions (diameter, wall thickness and length) of the tubes can be controlled in our fabrication process. The gold particles are deposited on the tubes by means of a modified deposition-precipitation method in HAuCl4 solution under controlled concentration of the solution. We show that by adjusting the fabrication conditions, we can obtain a high deposition density of the gold particles over the nanotube surface (over 90% coverage percentage ) and also have good control over the size of the gold nanoparticles (<5 nm). We show that there is an increase in particle size upon increasing the deposition period. The samples have been characterized by means of scanning and transmission electron microscopy. The optical and preliminary catalytic properties of such gold-supported Titania nanotubes will also be reported.

4:06PM X26.00009 Novel Fabrication and Enhanced Photosensitivity of Selenium Filament Arrays by Optical-Fiber Thermal Drawing, DAO SHENG DENG, N. ORF, A. ABOURADDY, Y. FINK, Massachusetts Institute of Technology — Structures with high aspect ratio and nanometer cross-sectional dimensions have been the subject of recent studies. These nanometer-scale wire structures are typically processed through a bottom-up approach that yields limited wire lengths lacking global orientation and presenting challenges to handling and electrical contacting. Here, we report a novel physical phenomenon in which a cylindrical shell undergoing a scaling process evolves into an ordered array of filaments upon reaching a characteristic thickness. We propose a fluid front instability mechanism to account for the observed phenomena. The fleeting evolution of fluid breakup from a thin film to a filament array is captured in the frozen state by a thermal drawing process which results in extended lengths of solid sub-100nm filaments encapsulated within a polymer fiber. Furthermore, we demonstrate that the electrical connectivity of centimeter-long filament arrays to external circuitry is readily achieved by contacting the fiber ends, allowing one to study their electrical and optoelectronic properties. Enhanced photosensitivity of filaments is observed compared to a selenium film. This approach offers unique opportunities for fabrication of nanometer scale devices of unprecedented lengths allowing simplified access and connectivity.

4:18PM X26.00010 Self-assembled Au nanorods - polymer composites, HEUNG-SHIK PARK, OLEG LAVERNTOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, ASHISH AGARWAL, NICHOLAS KOTOV, Department of Chemical Engineering, University of Michigan — The unique optoelectronic properties of the anisotropic metallic nanorods (NRs) are of great interest because of their potential applications in biological sensing, solar energy conversion, cloaking devices, etc. In order to utilize NRs, tuning their properties and immobilizing NRs into polymer matrix are essential. We present a simple and universal process for formation of self-assembled nanorods polymer composite. This approach is based on the anisotropic electrostatic interaction between aggregates of chromonic molecules and NRs that lead to either end-to-end or side-by-side assembly of NRs. We discuss encapsulation of these structures with polymer matrices.

1Supported by AFOSR under MURI grant FA9550-06-1-0337.

4:30PM X26.00011 Focused Ion Beam Treatment of ZnO Nanowires, GAGIK SHMAVONYAN, State Engineering University of Armenia — We investigated vapour-liquid-solid-grown ZnO nanowires (NWs) on a Si substrate by SEM. SEM investigations show that there are single NWs and ensembles of NWs, among which we found straight and bend, perfect and non-perfect NWs, as well as NWs with clean surfaces and surfaces with the dark spots and features. After focused ion beam polishing we found that every NW has a clean homogeneous surface, which allow us to conclude that all those dark spots and surface features of the NWs really are just surface features. The focused ion beam milling gives information of the deeper interior of the NWs, i.e. buried structures within the NWs and whether those structures are propagating within the NWs. But also here we found that there are no buried structures inside the NWs and the dark spots and features are not propagating within the NWs, which leads to the result that the NWs are totally homogeneous. The sizes of the NWs were determined: the length is about 2-24 μm, and the width and height are about 200-500 nm.

1Author thanks Prof. Dr. Jens Falta and his group at the University of Bremen, Germany.
4:42PM X26.00012 Controlled Growth of Zinc Oxide Nanostructures for Applications, ABHISHEK PRASAD, ARCHANA PANDEY, YOKE KHIN YAP, Michigan Technological University — Zinc Oxide (ZnO) has proven to be a versatile functional material with promising properties. Here we discuss about the controlled growth and applications of various ZnO nanostructures including novel ZnO nanotubes (NTs) and nanosquids (NSqs). We use a conventional thermal CVD technique for the synthesis of ZnO nanostructures. We found that ZnO nanowires, nanobelts and nanocoms can be readily obtained by applying appropriate gas flow rates and growth temperatures. ZnO NTs and NSqs can be formed on the substrates when appropriate cooling rate was applied. These nanostructures were characterized using XRD, HRTEM, FESEM, Raman spectroscopy, and photoluminescence. Results show that ZnO nanostructures were single crystals in wurtzite structure. Among these ZnO NWs were found to be excellent electron field emitters and field effect transistors.

1Y. K. Yap acknowledges support from the DARPA (DAAD17-03-C-0115, through Army Research Laboratory).

4:54PM X26.00013 CO Gas Sensing with ZnO Nanowire Mat, SIRISHA CHAVA, CHRISTINE BERVEN, University of Idaho, DAQUING ZHANG, California State University — We report the electrical properties of a gas sensor constructed from mats of ZnO nanowires grown on sapphire substrate that shows a reversible response which is unique to CO exposure. The sensor is a two terminal design, where the terminals consist of two 25 µm diameter gold wires laid parallel on the nanowire mat. The individual nanowires have an average diameter of 50 nm with lengths of about 10 µm. The nanowire mat is about 20 µm thick and extends over an area of about 1 cm2. When exposed to Ar, CO2 or H2 no significant changes in the current-voltage behavior of the mat are observed. CO exposure results in approximately a three-fold increase in current. The response is reversible after evacuation. Typical currents when exposed to pure CO under room temperature without prior introduction to any other gas are in the range of 40 nA compared to non-exposed 15 nA. Growth technique of nanowires and comparative work will be discussed.

5:06PM X26.00014 Transparent Thin Film Transistors based on Pristine and Doped Indium Oxide Nanowires, PO-CHIANG CHEN, GUOZHEN SHEN, SAOWALAK SUKCHAROENCHOKE, CHONGWU ZHOU, University of Southern California, UNIVERSITY OF SOUTHERN CALIFORNIA TEAM — The key to the realization of transparent electronics is the development of transparent thin film transistors (TTFT) with good device performance, in terms of high device mobility, low temperature fabrication, and optical transparency. We present our work on the fabrication of high performance TTFTs using both pristine In2O3 nanowires and doped In2O3 nanowires. In2O3 nanowire TTFTs were made on glass and PET substrates with Al2O3 as gate insulator and ITO source/drain electrodes. These devices showed a transparency of about 80% and n-type transistor performance. The device characteristics exhibit a subthreshold slope of 0.2 V/dec, a current on/off ratio of 106, and a field-effect mobility of 514 cm2/V−1S−1. We also fabricated TTFTs wbuilt on Arsenic-doped In2O3 nanowires with a field-effect mobility of 1,183.8 cm2/V−1S−1 without any post-treatments. In addition, we integrated TTFTs with organic light emitting diode (OLED) to make an active matrix organic light emitting diode (AMOLED) display, and thus made an animation by controlling the OLED light output.

5:18PM X26.00015 Studies of Surface Exciton Polaritons in Nano-Materials by Electron Energy-Loss Spectroscopy, C.H. CHEN, Center for Condensed Matter Sciences, National Taiwan University, C.T. WU, Department of Materials Science and Engineering, National Taiwan University, M.W. CHU, L.C. CHEN, Center for Condensed Matter Sciences, National Taiwan University, C.W. CHEN, Department of Materials Science and Engineering, National Taiwan University, K.H. CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — Surface plasmon polaritons (SPPs), which normally occur in the optically metallic spectral regime, are collective charge density oscillations of conduction electrons at the surface of metals. In sharp contrast to SPPs, the excitations of surface exciton polaritons (SEPs), which are collective oscillations of delocalized excitons at the surface of semiconductors or insulators, have been shown to be correlated with distinct excitonic onsets (interband transitions) in these materials. Using electron energy-loss spectroscopy (EELS) with a 2-A electron probe in the near-field geometry and energy-filtered spectral imaging in real space, we have unambiguously demonstrated the existence of the SEP excitations on the surfaces of GaN and ZnO nanorods at energies near the interband transitions.

Thursday, March 19, 2009 2:30PM - 5:30PM – Session X27-FlAP: Optoelectronic Devices and Applications 329

2:30PM X27.00001 Optical Fiber Tapers for Characterization of Novel Photonic Crystal Devices, JENNA HAGEMEIER, Physics Department, University of California, Santa Barbara, JAN GUDAT, Huygens Laboratory, University of Leiden, The Netherlands, SUSANNA THON, Physics Department, University of California, Santa Barbara, DIRK BOUWMEESTER, Physics Department, University of California, Santa Barbara and Huygens Laboratory, University of Leiden, The Netherlands — Optical fiber tapers are a useful tool for near-field spectroscopy of solid state devices. There are advantages to using fiber tapers rather than other waveguides because they can be moved spatially with respect to the device being studied, a single taper can be used for both pumping and data collection, and they can be used to probe bare cavities. The experimental procedures and challenges for building these microl-scale tapers will be discussed, as well as their uses for probing new kinds of photonic crystal cavities.

2:42PM X27.00002 Temporal Wavelength Multiplexing of a Quantum Cascade Laser, FATIMA TOOR, AMIRALI SHANECHI, JIANXIN CHEN, CLAIRE GMACHL, Electrical Engineering, Princeton University — Quantum cascade (QC) laser based sensor systems in the mid-infrared wavelength range (3-30 µm) have applications in environmental, industrial and medical trace gas sensing. QC laser-based spectroscopic techniques have been developed by several research groups. However, more research work is needed to make these techniques more compact and field deployable. One approach to compactness is to have spectral versatility from a single device. Here we report work on a QC laser based system that is both temporally and wavelength multiplexed, that is, it can emit two different wavelengths at two alternate time slots. A bi-directional and multi-wavelength QC laser source that emits at 10.2 µm wavelength for positive polarity current and 8.6 µm for negative polarity current is used. A system is designed so that a single pulsed current source is the input to a pulse-alternator circuit that flips the polarity of every other pulse. The output of the circuit is connected to the bi-directional and multi-wavelength QC laser to emit two different wavelengths for alternate pulses. Contributions by Gary Shu at the beginning of the work are acknowledged.

1This work is supported in part by MIRTHE (NSF-ERC).
3:06PM X27.00004 Electrically Pumped Quantum Post Vertical Cavity Surface Emitting Lasers, HYOCHUL KIM, MATTHEW RAKHER, DIRK BOUWMEESTER, Physics Department, University of California Santa Barbara, PIERRE PETROFF, Materials Science Department, University of California Santa Barbara — Quantum dot (QD) lasers based on high quality, small mode volume microcavities have shown low lasing current threshold. A novel MBE grown self assembled nanostructure, the quantum post (QP) is also a very good candidate as a gain medium for low threshold lasing. As opposed to the QD laser, the delta function density of states in the QP is associated with multiple vertically and laterally confined states. In addition, QPs have a large carrier capture cross section. We demonstrate very low threshold electrically pumped lasing in oxide apertured vertical cavity surface emitting lasers (VCSELs) with QPs as the active medium and compare their characteristics with similar structure with QDs as the active gain medium.

3:18PM X27.00005 In situ Contact Resistance Evaluation of 2.6-2.9 THz Quantum Cascade Lasers, NEELIMA CHANDRAYAN, KRONTIP TREMKIOA, JIN LI, XIFENG QIAN, SHIVASHANKAR VANGALA, WILLIAM GOODHUE, Photonics Center, Dept. of Physics, UMass Lowell, ANDRIY DANYLOV, JERRY WALDMAN, ROBERT GILES, Sub-millimeter Wave Technology Lab, Dept. of Physics, UMass Lowell, WILLIAM NIXON, U.S. Army National Ground Intelligence Center — The fabrication of THz Quantum Cascade Lasers (QCL) requires a strong understanding of the two electrical contacts of the device. Contact resistance as well as contact/semiconductor interdiffusion properties must be designed to minimize series resistance, free carrier absorption, and e-e scattering. Here, in situ measurement of contact resistance using Transmission Line Measurement (TLM) pads has been implemented in the fabrication of 2.6-2.9 THz quantum cascade lasers. The measurement of contact resistances as part of device processing also verifies the correct etch depth of laser structure, uniformity of the etching, and the ohmic nature of the contacts. For example, the procedure has been used to successfully fabricate 2.93 THz lasers with 5 mW of continuous wave output power.

3:30PM X27.00006 Magnetic Field Assisted sub-THz Quantum Cascade Lasers, A. WADE, Y. KIM, D. SMIRNOV, National High Magnetic Field Laboratory, S. KUMAR, Q. HU, Massachusetts Institute of Technology, B.S. WILLIAMS, University of California, Los Angeles, J. RENO, Sandia National Labs — In THz QCLs radiative transitions take place between closely-spaced 2D electronic subbands (1THz ~ 4meV) of a multi-QW semiconductor system. THz quantum cascade lasers now cover the frequency range from 1.2 THz to 5 THz, though cryogenic cooling is still required. Further progress towards the realization of devices emitting at longer wavelengths (sub-THz QCLs) and higher temperatures may be realized in a system with additional lateral confinement. Here we use strong magnetic fields to achieve quasi-0D confinement in THz QCL based on the resonance phonon design. We studied two designs: (a) 2-well injector/2 well active region, emitting at 3 THz at B=0; and (b) 1-well injector/3-well active region, emitting at 2 THz at B=0. T by applying the appropriate electrical bias and strong magnetic fields, we achieved laser emission at 0.8-0.9 THz at B=16 T [1], and 0.6 THz at B=17 T, from devices a and b respectively. The ability to achieve sub-THz lasing is due to magnetic field enhanced population inversion in a quasi-0D QCL.

3:42PM X27.00007 Conducting a wide-range single-transverse mode operation in a commercial multi-mode VCSEL by beam-profile transferred optical feedback1, CHUAN-PI HSU, TSU-CHIANG YEN, Department of Physics, National Sun Yat-sen University, DA-LONG CHENG, Department of Computer and Communication, SHU-TE UNIVERSITY, WANG-CHUANG KUO, Department of Physics, National Sun Yat-sen University — In this research, a beam-profile transferred optical feedback (BTOF) method was employed to conduct a wide range single-transverse mode operation of a commercial multi-mode VCSEL. In BTOF, a spatial modulation optical system was used to reconfigure the spatial distribution of the feedback beam, and to control the laser’s transverse mode. Experimental results indicated that, over a range of about 8.7 times of the laser’s threshold current, BTOF could conduct the laser to output a single-transverse mode with high spectral purity and low intensity noise. While, without optical feedback, the solitary laser exhibited a multi-mode output with a complicated variation in mode distribution as the laser’s current was tuned. More special features of BTOF will be presented in the report.

Supported by NSC of R.O.C. under grand No. NSC 96-2112-M-110-008-MY2

3:54PM X27.00008 Single mode operation in ultra-short cavity Quantum Cascade lasers1, RICHARD CENDEJAS, Princeton University, WENDY SANCHEZ-VAYNSHTEYN, City University of New York, DONGXIA QU, CLAIRE GMACHL, Princeton University — Single-mode continuous wave operation of a A=5.3 μm Quantum Cascade laser (QCL) is achieved through the systematic shortening of the cavity length of ridge-waveguide QCLs with wavelength of emitting from 800 to 1000 μm. Increasing mirror loss was mitigated with highly reflective metallic facet coatings. With smaller cavity lengths, the power consumption of an ultra-short cavity QCL of 110 μm is ~250 mW at 80K, or about 20 times lower than conventional QCLs. Shortening the cavity length increases the free spectral range of the longitudinal modes placing the side modes at the edge of the gain profile, thus deliberately reducing the number of lasing modes until single-mode operation is achieved. The dominant mode is placed on the gain peak via temperature tuning, increasing the gain margin between the dominant and side modes, further increasing the single-mode current range. Amplified spontaneous emission spectra at various temperatures show that an initial gain margin increase from 1.5:1 to 2:1 doubles the single-mode current range. Ultra-short cavity QCLs with lengths of 110 μm are shown to operate single mode with the best device having a 10 cm⁻¹ single-mode continuous tuning.

Work supported in part by MIRTHE NSF-ERC

4:06PM X27.00009 Correlated Photon Noise at Threshold of an Interband Cascade Laser, PATRICK FOLKES, Army Research Laboratory — We report the observation of correlated photon fluctuations at threshold of an interband cascade laser at 30 K and 100 K. Away from threshold, the laser exhibits a frequency-independent photon noise spectral density. The correlated photon noise is manifested by fluctuations in the low-frequency photon noise spectral density at certain frequencies over a narrow range of current near threshold. Concurrently, we observe the emergence and growth of the lasing mode over the same current range. The data indicates that the correlated photon noise is caused by the onset of laser coherence.
4:18PM X27.00010 Effect of free carrier absorption on the efficiency of nitride devices.
EMMANOUL KIOUPAKIS, University of California, Santa Barbara, ANDRE SCHLEIFE, IFTO, Friedrich-Schiller-Universitaet Jena, PATRICK RINKE, University of California, Santa Barbara, FRIEDHELM BECHSTEDT, IFTO, Friedrich-Schiller-Universitaet Jena, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Indium gallium nitride alloys are successfully being used in the fabrication of optoelectronic devices, such as light emitting and laser diodes, in the green to ultraviolet part of the optical spectrum. The wider application of these devices, however, is limited by their reduced efficiency in the green part of the spectrum. Several mechanisms have been suggested as the cause of this efficiency loss, such as Auger recombination and free carrier absorption. We use the band structure and density-matrix elements from highly accurate many-body perturbation theory calculations in the GW approach (P. Rinke et al., Phys. Rev. B77, 075202 (2008)) to determine the optical absorption coefficient due to free carriers in InGaN. From this we obtain the corresponding photon mean free path and examine the role of free carrier absorption as a possible energy loss mechanism at high carrier concentrations. The computed values indicate that the effect is weak in light emitting diodes but it may become relevant for laser devices that operate at higher current densities.

4:30PM X27.00011 Light Emission Polarization Properties of a-plane InGaN/GaN Quantum Wells.
HUNG-HSUN HUANG, YUH-RENN WU, Graduate Institute of Photonics and Optoelectronics, National Taiwan University — This paper discusses the optical characteristics for nonpolar a-plane InGaN/GaN quantum wells (QWs) with different indium compositions, QW well widths, and injection carrier densities. We compared it with the results of the conventional c-plane QWs and analyzed the characteristics of optical anisotropy polarization in (110)-oriented wurzite a-plane InGaN-based QWs. A self-consistent Poisson, Schrodinger, and many-body-perturbation theory calculations (density-functional and many-body-perturbation theory), in which individual loss processes can explicitly be isolated, that Auger recombination is a key loss mechanism in wurzite InGaN. Auger recombination had previously been proposed by Shen et al. [1] as a loss mechanism in optically pumped InGaN LED devices, but it is difficult to discriminate between different radiationless processes experimentally. We examine two different mechanisms — inter- and intra-band recombination — that affect different parts of the spectrum. In the blue to green spectral region and at room temperature the Auger coefficient can be as large as 2x10^{-10} cm^2/s -1 and in the infrared even larger. Since Auger recombination scales with the cubic power of the free-carrier concentration it becomes an important non-radiative loss mechanism at high current densities. [1] Shen et al., Appl. Phys. Lett. 91, 141101 (2007).

4:42PM X27.00012 Auger recombination rates in nitrides from first principles.
PATRICK RINKE, KRIS T. DELANEY, CHRIS G. VAN DE WALLE, University of California at Santa Barbara, CA 93106 — Indium gallium nitride (InGaN) alloys are successfully being used for light emitting and laser diodes in the green to ultraviolet part of the spectrum, but increases in internal quantum efficiency (IQE) are still required to allow broader applications. The IQE of InGaN devices is limited by loss mechanisms that, at high drive currents (i.e., high carrier concentrations) lead to a decrease in IQE, a phenomenon commonly referred to as "efficiency droop". We demonstrate by means of rigorous first-principles calculations (density-functional and many-body-perturbation theory), in which individual loss processes can explicitly be isolated, that Auger recombination is a key loss mechanism in wurtzite InGaN. Auger recombination has previously been proposed by Shen et al. [1] as a loss mechanism in optically pumped InGaN LED devices, but it is difficult to discriminate between different radiationless processes experimentally. We examine two different mechanisms — inter- and intra-band recombination — that affect different parts of the spectrum. In the blue to green spectral region and at room temperature the Auger coefficient can be as large as 2x10^{-10} cm^2/s -1 and in the infrared even larger. Since Auger recombination scales with the cubic power of the free-carrier concentration it becomes an important non-radiative loss mechanism at high current densities. [1] Shen et al., Appl. Phys. Lett. 91, 141101 (2007).

4:54PM X27.00013 Enhancement of terahertz output power in terahertz parametric oscillator with recycled pump beam.
DONG HO WU1, Naval Research Laboratory, TOMOFUMI IKARI2, Temple University — In the terahertz parametric technique the pump beam is used only once, and then dumped, regardless that the dumped pump beam still has substantial laser energy. So the energy efficiency of the technique is low. This paper reports a new parametric technique in which we recycle the pump beam (instead of dumping it) in order to increase the efficiency and enhance the terahertz beam output. Our experiments, in which we used a doped LiNbO3 crystal with 5% MgO, indicate that the terahertz beam output increases almost five times magnitude for a terahertz parametric oscillator with recycled pump beam.

5:06PM X27.00014 Electro-optic sensors for high power microwave measurements.
ANTHONY GARZARELLA, DONG HO WU, Naval Research Lab — Nonperturbative measurements of high power microwave fields utilizing electro-optic (EO) field sensors are described. Conventional metallic-based field probes (such as dipole antennas) perturb the very fields they measure and typically saturate for field strengths exceeding ~1000 V/m. EO sensors are all-dielectric, have large intrinsic bandwidths (DC to THz), and measure the true waveform of the field noninvasively. Nonlinear EO crystals such as Lithium Niobate or Potassium Dideuterium Phosphate have half-wave retardation fields of the order 10^9 V/m, making them ideal for high power microwave applications. Initial field tests with our EO sensors revealed several sources of noise and instability which are normally not encountered in laboratory settings. In this presentation, we describe a newly-designed EO sensor and how it is configured to address the noise issues in high power microwave field tests. Using this improved sensor configuration, electric field measurements in the near and far field regions of a radiating microwave horn antenna are presented.

ALEX NEMIROSKI, KEITH BROWN, DAVID ISSADORE, ROBERT WESTERVETL, Harvard University School of Engineering and Applied Science, CHRIS THOMPSON, KEITH OBSTEIN, Harvard University Medical School, MICHAEL LAINE, Soltegic, LLC. — We have built a miniature wireless biosensor with fluorescence detection capability that explores the miniaturization limit for a self-powered sensor device assembled from the latest off-the-shelf technology. The device is intended as a remote medical sensor to be inserted endoscopically and remains in a patient’s gastrointestinal tract for a period of weeks, recording and transmitting data as necessary. A sensing network may be formed by using multiple such devices within the patient, routing information to an external receiver that communicates through existing mobilephone networks to relay data remotely. By using a monolithic IC chip with integrated processor, memory, and 2.4 GHz radio, combined with a photonic sensor and miniature battery, we have developed a fully functional computing device in a form factor compatible with insertion through the narrowest endoscopic channels (less than 3mm x 3mm x 20mm). We envision similar devices with various types of sensors to be used in many different areas of the human body.
2:30PM X28.00001 Quantitative investigation of magnetoelectric coupling in various forms of multiferroics, KEE HOON KIM, Seoul National University — Magnetoelectric susceptibility (MES) is probably the most direct way of estimating the magnitude of magnetoelectric coupling in many forms of multiferroic materials. However, the MES has been found in numerous existing magnetoelectric materials in broad field, frequency, and temperature ranges and their MES values have been tabulated [1]. With growing interest worldwide toward applications of magnetoelectric for novel memory and sensor devices, however, there have been ever-increasing demands to measure quantitatively the MES of multiferroic thin films. Yet, the measurements of thin film MES become challenging in spite of its large MES value because the magnetoelectric voltages, proportional to the film thickness, usually get too small to be measured reliably. Herein, we introduce a highly sensitive magnetoelectric susceptometer that can detect the charge variation down to \(\sim 10^{-17} \text{C}\) in a few gauss oscillating magnetic field. Using this specific setup, we could measure the MES of multiferroic thin films or single crystals with unprecedented accuracy and sensitivity in cryogenic (down to 2 K) and magnetic field (up to 9 T) environments. In this talk, we summarize a number of key results based on this technique; (1) MES of a 300 nm BiFeO\(_3\)-CoFe\(_2\)O\(_4\) nanopillar structure as well as that of a 250 nm BiFeO\(_3\) film and of a BiFeO\(_3\) single crystal. (2) MES of (Pb,Zr)TiO\(_3\)-NiFe\(_2\)O\(_4\) nanocomposite films, and (3) temperature- and field-dependent MES in representative multiferroic crystals/films including TbMn\(_2\)O\(_4\), GaFeO\(_3\), and Cr\(_2\)O\(_3\). In particular, we demonstrate that the MES of the film with the nanopillar structure is enhanced by approximately one order of magnitude reaching \(210^{12} \text{V/(Oe cm)}\) at room temperature, compared with those of a pure BiFeO\(_3\) film and a single crystal. Furthermore, based on detailed field and temperature dependent MES studies, we show that magnetoelectric coupling in TbMn\(_2\)O\(_4\) has been mediated and amplified by the large magnetoelastic effect. [1] G. A. Smolenskii and I. E. Chupis, Sov. Phys. Usp. 25, 475 (1982); F. W. Hehl et al. Phys. Rev. A 77, 022106 (2008).

3:06PM X28.00002 Magnetoelectric effects induced by domain walls, ANDREA SCARAMUCCI, University of Groningen, THOMAS KAPLAN, Michigan State University, MAXIM MOSTOVOY, University of Groningen — We explore the possibility to observe high-temperature multiferroic behavior in thin films of ordinary ferrimagnets. In thin films magnetostatic interactions induce periodic stripe domain patterns. We show that stripe domain patterns, stabilized by magneto-dipolar interactions, have ferroelectric properties similar to those of magnetic spirals in bulk materials. We studied behavior of domain patterns and the induced electric polarization in applied magnetic and electric fields using mean field approximation and Monte Carlo simulations. We find a sharp increase in dielectric constant and ferroelectric polarization at the critical field, induced by both magnetic and electric field. We studied the domain walls in conical spiral multiferros, where magnetization \(M\) consists with the electric polarization \(P\) induced by the cylindrical spiral. The structure of these domain walls explains the conservation of \(P \times M\) recently observed in CoCr\(_2\)O\(_4\) as well as the magnetic field dependence of the polarization vector \(P\) in ZnCr\(_2\)Se\(_4\).

3:18PM X28.00003 Large electric polarization in high pressure synthesized orthorhombic manganites \(\text{RMn}_\text{O}_3\) (\(R=\text{Ho, Tm, Yb, and Lu}\)) by using the double-wave PE loop measurements, Y.S. CHAI, Y.S. OH, N. MANIVANNAN, Y.S. YANG, KEE HOON KIM, XMPL, Seoul National University, S.M. FENG, L.J. WANG, C.Q. JIN, Institute of Physics, Chinese Academy of Science — The magnitude of electric polarization via the conventional pyroelectric current and/or PE loop measurements often is ambiguous due to resistive components of the sample. To avoid this, a new technique called the double-wave method has been developed [1], in which only hysteretic PE components can be measured. Using this technique, we have measured the ferroelectric polarization of the orthorhombic \(\text{RMn}_\text{O}_3\) (\(R=\text{Ho, Tm, Yb, and Lu}\)) synthesized at high pressure. Large remnant polarization \(P_r\) up to 920 \(\mu\text{C/cm}^2\) is observed at 10 K for LuMn\(_3\)O\(_7\). Furthermore, the \(P\) vs. temperature data from the PE loop has shown consistency with that measured through the pyroelectric current measurements, supporting a theoretical prediction of large polarization in the \(E\)-type spin structure in this system [2]. We also discuss the influence of thermal histories on the ferroelectric domain dynamics and possible internal bias field effects originating from oxygen vacancies in \(\text{RMn}_\text{O}_3\). [1] M. Fukunaga, et al. J. Phys. Soc. Jpn. 77, 064706 (2008). [2] I. A. Sergienko, et al. Phys. Rev. Lett., 97, 227204 (2006).

3:30PM X28.00004 Chemical engineering of the critical magnetic field for switching ferroelectricity in multiferroic hexaferrites, SAE HWAN CHUN, YISHENG CHAI, SO YOUNG HAM, DEEPSHIKA JAIWAL-NAGAR, DONG HAK NAM, YOON SEOK OH, INGUY KIM, BEOM SUNG LEE, KEE HOON KIM, FPRD, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, KYUNG TAE KO, JAE HOON PARK, Department of Physics, POSTECH, Pohang 790-784, Korea, JAE-HO CHUNG, Department of Physics, Physics Korea, Seoul 136-713, Korea — Multiferroics wherein the magnetic and ferroelectric order parameters coexist with their large cross-coupling effects have promising application potentials for multifunctional devices. To realize various technical exploitations, not only the capability of switching ferroelectricity with low magnetic field but also the tunability of the critical magnetic field \((H_c)\) for the switching is essential. Herein, we report our discovery of a novel chemical route to engineer \(H_c\) in a low field regime in the multiferroic hexaferrite system and discuss its mechanism.

3:42PM X28.00005 Ferroelectric and magnetic properties of multiferroic BaCoF\(_3\) thin films, TRENT JOHNSON, FELIO PEREZ, DAVID LEDERMAN, West Virginia University — Thin films of BaCoF\(_3\) have been successfully fabricated by molecular beam epitaxy and e beam technique on sapphire substrate (110), with a buffer layer of palladium grown using sputtering dc in argon atmosphere. Here we investigated the structural, morphological and ferroelectric properties were analyzed by means of various characterization techniques. The x-ray patterns showed that the films were oriented, but RHEED showed that the films were polycrystalline in the plane. AFM images showed a relatively granular surface. Measurements of the dielectric polarization showed that the films were ferroelectric at room temperature. The effect of magnetic fields on the ferroelectric properties at cryogenic temperatures will be described.

This work is supported by National Science Foundation (grant EPS-0314742) and the WVNano Initiative at West Virginia University.

3:54PM X28.00006 All thin film magnetoelectric magnetic field sensors, PENG ZHAO, University of Maryland, College Park — We have fabricated prototype ac magnetic field sensors operating at room temperature based on all thin film ME devices showing strong magnetoelectric (ME) coupling. The ME layers consist of a sol-gel derived Pb\((\text{Zr}_{0.52}\text{Ti}_{0.48})\)TiO\(_3\) (PZT) film and a dc magnetron sputter deposited magnetostrictive Fe\(_{72}\)Ga\(_{28}\) (FeGa) film. The bilayer structures are prepared on micromachined Si wafers, and the laser cutting technique is used to release and isolate the cantilevers for optimization of the sensor performance. The PZT layer and the FeGa layer couple via the piezoelectric \(d_{33}\) mode and the corresponding ME coupling coefficient is as high as \(\pm 2\text{ V/} (\text{Oe cm})\) for a lateral dimension of 1 mm\(^2\) device at the mechanical resonant frequency of 333 Hz of a Si cantilever. The soft magnetic FeGa film requires dc bias magnetic field of around 90 Oe to operate the thin film ME device. The coupling between the PZT and the FeGa films is remarkably improved by depositing a 40 nm thick Pt intermediate layer. The clamping effect on the ME coupling is dramatically reduced by back-etching the Si cantilever down to 35 \(\mu\)m thick. The present work indicates presence of robust ME coupling in microfabricated multilayer thin film ME devices.

This work is done with collaboration with Zhenli Zhao, Richard Suchoski, Scott Mathews, Chen Gao, Manfred Wuttig, and Ichiro Takeuchi. This work is funded by NSF, Mosaic at UMD and ARO.
4:30PM X28.00007 Magnetic anisotropy modulation of magnetite in Fe$_3$O$_4$/BaTiO$_3$(100) epitaxial structures. CARLOS A.F. VAZ, JASON HOFFMAN, AGHAM POSADAS, CHARLES AHN, Yale University and Center for Research on Interface Structures and Phenomena (CRISP) — Temperature dependent magnetometry and transport measurements on epitaxial Fe$_3$O$_4$ films grown on BaTiO$_3$(100) single crystals by molecular beam epitaxy show a series of discontinuities that are attributed to changes in the magnetic anisotropy induced by strain in the different crystal phases of BaTiO$_3$. High resolution x-ray diffraction measurements show that the magnetite film is under tensile strain at room temperature, which is ascribed to the lattice expansion of BaTiO$_3$ at the cubic to tetragonal transition, indicating that the magnetite film is relaxed at the growth temperature. From the magnetization versus temperature curves, the variation in the magnetic anisotropy is determined and compared with numerical estimates for the magnetoelastic anisotropies. In particular, the tensile strain in the Fe$_3$O$_4$ films is shown to give rise to a strong perpendicular magnetic anisotropy, as observed experimentally. These results demonstrate the possibility of using the piezoelectric response of BaTiO$_3$ to modulate the magnetic anisotropy of magnetite films.

4:42PM X28.00008 Enhanced power output from a magnetically coupled piezoelectric cantilever. JI-TZUOH LIN, University of Louisville, BARCLAY LEE, DuPont Manual High School, BRUCE ALPHENAAR, University of Louisville, WALTER JONES, DEIRDRE ALPHENAAR, Gencsape, Inc. — Piezoelectric cantilevers have been widely studied for energy scavenging applications, but suffer from poor output power outside of a narrow frequency range near the cantilever resonance. Here, we demonstrate how power output can be enhanced by applying a simple passive external force. A symmetrical and repulsive magnetic force is applied to a piezoelectric cantilever beam to compensate the cantilever spring force. The raised and compensated spring potential introduced by the magnetic coupling is found to broaden the frequency response without altering the resonant frequency or introducing damping at resonance. Furthermore, the modified cantilever responds chaotically outside of the resonant frequency, causing increased voltage output across a large spectral region. The total voltage output across the spectrum increases between 31% and 87%. Model calculations support these results.

4:54PM X28.00009 Quantitative determination of the enhanced magnetoelectric. YOUNG HOON KIM, Dept. of Physics and Astronomy, Seoul National University, STEVEN P. CRANE, R. RAMESH, University of California, Berkeley, SEONGSU LEE, S-W. CHEONG, Rutgers University — With growing interest worldwide toward applications of multiferroic materials for novel memory and magnetic sensor devices, there have been numerous efforts to synthesize multiferroic thin films with large magnetoelectric coupling. Yet, quantitative information on the strain in the different crystal phases of BaTiO$_3$ is still lacking because it is difficult to measure a reduced magnetoelectric signal due to a tiny thickness. In the present work, we have determined quantitative MES for a 300 nm BiFeO$_3$/CoFe$_2$O$_4$ nanostructure, 250 nm BiFeO$_3$ film, and BiFeO$_3$ single crystal with our highly sensitive magnetoelectric susceptometer operating in cryogenic (down to 2 K) and high magnetic field, $H$, (up to 9 T) environments. We find that the MES of the BiFeO$_3$/CoFe$_2$O$_4$ nanostructure shows a typical anti-symmetric shape with DC magnetic field up to 340 K, as expected in the magnetoelectric coupling mediated by strain between piezoelectric and magnetostrictive materials. At room temperature, the transverse MES of the nanostructure shows a maximum of $2 \times 10^{-10}$ V/m at low $H = 6$ kOe. Our results also demonstrate that the MES value of the nanopillar structured film is enhanced by approximately one order of magnitude than that of pure 250 nm BiFeO$_3$ film and BiFeO$_3$ single crystal.

5:06PM X28.00010 Epitaxial complex oxide tunnel barriers. JUNWOO SON, POUYA MOATAKEF, JOEL CAGNON, SUSANNE STEMMER, University of California, Santa Barbara — Tunnel junctions with complex oxide thin film barriers are of interest for studies of the critical thickness of ferroelectricity, of phonon modes in ultrathin films and of traps in inelastic tunneling spectroscopy. We show that high-quality epitaxial SrTiO$_3$ and BaTiO$_3$ tunnel barriers can be grown on Pt bottom electrodes. Coherent, epitaxial Pt films with roughness of less than a unit cell were grown on (001) SrTiO$_3$ to serve as bottom electrodes for epitaxial SrTiO$_3$ and BaTiO$_3$ tunnel barriers. All interfaces were atomically abrupt as confirmed by atomic resolution Z-contrast imaging. The IV characteristics were non-linear, demonstrating good insulating properties. For the SrTiO$_3$ barriers and voltage sweeps up to $\pm 0.5$ V, the measured tunnel current was independent of the sweep direction. At low biases, dynamic conductance curves showed a symmetrical parabolic shape around the origin in both resistance states. At high bias, deviation from the ideal tunnel behavior was observed. A large increase of the tunnel conductance occurred above a minimum positive bias. A dramatic decrease of tunnel conductance occurred for a large negative bias, indicating bipolar switching. We show the contributions to the resistive switching. Phonon modes and traps are determined using inelastic tunneling spectroscopy with both paraelectric and ferroelectric tunnel barriers.

Thursday, March 19, 2009 2:30PM - 5:18PM — Session X29 GMAG DMP FLAP: Focus Session: Current Induced Dynamics in Magnetic Tunnel Junctions and Spin Waves

2:30PM X29.00001 Influence of electron-magnon scattering on spin transfer torque in magnetic tunnel junctions. AURELIEN MANCHON, SHUFENG ZHANG, University of Arizona — Manipulating the magnetization direction using spin transfer torque in magnetic tunnel junctions (MTJs) has been one of the most important challenges in spin electronics for the past five years. Elastic tunneling theories show that the torque possesses two components, one being mainly linear in bias voltage whereas the other shows a quadratic bias dependence. These theoretical results have been recently confirmed by “spin-diode” experiments [1]. However, the validity of the elastic tunneling has been questioned by two experimental studies [2]. These studies show that the bias dependence of the out-of-plane torque can be dramatically different from the elastic quadratic dependence. Using the Transfer Hamiltonian formalism, we study the influence of interfacial electron-magnon scattering on the bias dependence of the spin transfer torque. We show that the bias dependence can strongly affect the bias dependence of the spin transfer torque in agreement with the recent experimental studies [2]. [1] J. C. Slonczewski, J. Phys. Condens. Matter 11, A509-11 (1999). [2] S. Petit, et al., Phys. Rev. Lett. 98, 077203 (2007); Z. Li, et al., Phys. Rev. Lett. 100, 246602 (2008).

2:42PM X29.00002 Macrospin model of incubation delay due to field-like spin transfer torque. SAMIR GARZON, YAROSLAV BAZALY, RICHARD A. WEBB, University of South Carolina, MARK COVINGTON, SHEHZAAD KAKA, Seagate Research, THOMAS M. CRAWFORD, University of South Carolina — While extensive measurements have tested the validity and limitations of the macrospin model with Slonczewski’s spin transfer torque in metallic spin valves, recent experiments with magnetic tunnel junctions (MTJs) have reported an additional “field-like” or “perpendicular” spin torque. The observed field-like torques generally agree with theoretical predictions, but some controversies remain: frequency domain measurements at low voltages and switching current measurements at large voltages report contradictory signs for the field-like term. Here we show that the absence of pre-switching oscillations (“incubation delay”) reported in magnetic tunnel junctions can be explained within the macrospin model by a sizable field-like component of the spin-transfer torque. Furthermore, we propose that measurements of the voltage dependence of the tunnel junction switching time in the presence of external easy axis magnetic fields can be used to determine the magnitude and voltage dependence of the field-like torque over a broad range of voltages.

1This work was supported by NSF (DMR-0704182) and DOE (DEFG02-06ER46307).

2This work was supported by NSF (DMR-0802318) and DOE (DE-FG02-08ER46628).
H. Kubota et al., IEEE Trans. Mag.  

d\tau was initially reported by two groups. After the correction is applied, we measure consistent values of \( dV/dI \) of the spin torque. In the case of an applied field along the easy axis, which can be attributed to the differences in the precession axis and switching barriers as well as effects of thermal fluctuations. We will also report results of single-shot transport measurements in the regime of spin-torque-driven steady-state precession.

3:06PM X29.00004 Bias and Angular Dependence of Spin-Transfer Torque in Magnetic Tunnel Junctions, C. Wang, Y.-T. Cui, R.A. Buhrman, D.C. Ralph, Cornell University, Ithaca, NY 14853, DANIELE MAURI, JORDAN A. KATINE, Hitachi Global Storage Technologies, San Jose Research Center, San Jose, CA 95135 — We present single-shot time domain resistance measurements of spin-transfer-driven dynamics in CoFeB/MgO/CoFeB tunnel junctions. In the regime of thermally-activated current-driven switching, we have sufficient sensitivity to resolve the pattern of resistance oscillations caused by the magnetic dynamics leading up to switching. When an in-plane hard-axis magnetic field is applied, within a short interval before the switching instant the resistance oscillations show a steadily-increasing amplitude, qualitatively consistent with expectations for large-angle precession in a single macrospin model, although the oscillation amplitude can vary between individual switching events. Moreover, the oscillation rate is observed to be absent in the case of an applied field along the easy axis, which can be attributed to the differences in the precession axis and switching barriers as well as effects of thermal fluctuations. We will also report results of single-shot transport measurements in the regime of spin-torque-driven steady-state precession.

3:18PM X29.00005 Effect of asymmetry on the bias dependence of spin torque in magnetic tunnel junctions, N. KIOUSSIS, Y.-H. TANG, ALAN KALITSOV, California State University, Northridge — The switching of magnetic states in magnetic tunnel junctions (MTJ) by spin-polarized current via the spin torque has been the subject of intensive theoretical and experimental researches. One outstanding question which remains unresolved and controversial is the bias dependence of field-like spin torque, \( T_{\text{per}} \), parallel to the plane of the two magnetizations. In this study, we show that bias behavior of \( T_{\text{per}} \) can change dramatically with the asymmetry in the ferromagnetic electrodes from purely quadratic with negative curvature in agreement with Kubota’s experimental results [1], to linear with sign reverse with bias in agreement of Li’s observation [2], and finally to quadratic but with positive curvature in agreement with Sankey’s experiments [3]. These results suggest that the asymmetry due to the amorphous alloys may cause the discrepancy in the bias dependence of \( T_{\text{per}} \) in experimental findings [1-3]. Moreover, our results have important practical applications for MRAM devices, since the magnetic configurations of MTJ can be tuned by external bias and without the application of external magnetic field. This work is supported by NSF PREM Grant No. DMR-0011656. [1] J. Kubota et al., Nature Phys. 4, 37 (2008) [2] Z. Li et al., Phys. Rev. Lett. 100, 246602 (2008) [3] J. C. Sankey et al., Nature Phys. 4, 67 (2008).

3:30PM X29.00006 Voltage dependence properties of ballistic spin currents and spin torques in magnetic tunnel junctions, MAIRBEK CHSHIEV, SPINTEC, CEA/CNRS, Grenoble, France / MINT Center, University of Alabama, AL, USA — Interest in spintronics [1] has been strongly accentuated by the discovery of current induced magnetization switching caused by spin transfer torques (STT) [2]. Among the most favorable candidate systems for the realization of STT-based spintronic devices are epitaxial magnetic tunnel junctions (MTJ) [3]. Here we present a systematic study of voltage-induced STT in MTJs and provide an insight into the nature of its voltage behavior by investigating the properties of membrane spin currents [4,5]. We demonstrate that the band filling has a dramatic impact on voltage dependence properties of both STT components, tunnel magnetoresistance (TMR) as well as on equilibrium interlayer exchange coupling [5]. Both in-plane (Slonczewski) and perpendicular-to-plane (field-like) STT components demonstrate a wide range of nontrivial behavior as a function of applied voltage [4,5]. The explanation is given in terms of the spin and charge current dependence on the interplay between evanescent states in the insulator and the Fermi surfaces of the ferromagnetic electrodes comprising the MTJ [5]. In particular we show that in ballistic regime the field-like torque is an even parity function of applied voltage while the parallel torque may exhibit a range of behavior [4,5]. Recent experiments [6] are in agreement with these predictions. Calculations are based on the non-equilibrium Green functions technique.

4:06PM X29.00007 Excitation of magnetization dynamics in patterned thin films using surface acoustic waves, A. BARUTH, S. ADENWALLA, University of Nebraska - Lincoln — The investigation of magnetization dynamics often involves the application of magnetic field or light pulses on very short time scales. Here we outline an alternative method that utilizes the changes in magnetic anisotropy associated with magneto-elastic strain. Surface Acoustic Wave (SAW) transducers are readily available at high frequencies (>10GHz), and provide an ideal method for straining thin film magnetic elements. SAWs propagate across a piezoelectric substrate, alternately compressing and expanding the surface with a wavelength on the order of a few millimeters. The periodicity of the interdigital transducer (IDT) that produces the SAW. Patterning thin film magnetic nanostructures at a spacing identical to the SAW wavelength ensures that all elements will be in phase as the SAW passes through. Passage of the SAW through a magnetic element leads to expansion and compression along the SAW propagation direction dynamically altering the easy axis of magnetization at ultra high frequencies. The subsequent dynamics can be probed using the Kerr effect. Using an IDT of 100 fingers operating at 87.2 MHz with realistic insertion losses, an array of 30 mm thick, 10x20pm2 rectangular Co bars require voltages of ~3.3V to fully switch the magnetization from the easy to hard axis without the application of an external field. Funded by NSF-MRSEC DMR-0820521.

4:18PM X29.00008 Spin Wave Quantization by the Stripe Domain Structures in a Continuous Film, CHUN-YEOL YOU, SEUNG-SOEK HA, JUNGBUM YOON, SUKMOCK LEE, Dept. of Phys. Inha University, MYUNG-HWA JUNG, Dept. of Phys. Sogang Univ., YOUNG KEUN KIM, Deparment of Materials Science and Engineering, Korea University — Abnormal field dependence and dispersion relations of spin wave excitations in the Brillouin light scattering were observed in a continuous CoFeSiB film. The observed spectra are similar to spin wave quantization in laterally-confined magnetic structures such as arrays of magnetic nanowires. In the array of nanowires, the propagating spin wave formed a standing wave due to the reflection from the geometrical confinement, boundaries of the nanowire, and the spin wave exciting modes are quantized. In our observation, the possible reflection source in the continuous CoFeSiB film is the regular stripe domain boundaries, domain walls. As evidence, we observed very regular stripe domain structures by magnetic force microscopy. In the low field region (11 kOe), the regular stripe domain patterns are formed and additional spin wave excitations are observed, while in the large field region, it behaves as usual continuous film. We believe that the regular domain wall acts as a scattering source of the spin wave, and it causes spin wave mode quantization.
range, 0.04 likely due to strong electron correlation effects. The various contributions to the heat capacity provide a detailed picture of the evolution of the phase-separated observations include a discontinuity in Debye temperature accompanying the percolation-type insulator-metal transition and a large electron mass enhancement, \( T \leq 1 \).

Mitchell (Argonne National Lab). Work supported by DoE and NSF.

are not required to explain the physical properties of these cobaltites. Co-authors: C. He, S. El-Khatib, J. Wu, (UMN), J.W. Lynn (NIST), H. Zheng, J.F. MITCHELL, University of California, Los Angeles, AJEY JACOB, Intel — To date, the spin-wave logic devices are seen promising for parallel data processing at high speed (Appl. Phys. Lett. 87, 153501 (2005), and Superlattices and Microstructures 38, 184 (2005)). However, there is no power gain with the current spin-wave logic devices, and the spin-wave cannot propagate a long distance because of the spin-wave dumping effect. All those will prevent the spin-wave devices from real applications. Here we report a spin-wave amplifier with a power gain that is controlled by the pumping power level. At the pumping power of 16 dBm at 2.6 GHz, the power gain is 6.4 dB and the frequency is 1.3 GHz. The amplifier is made from a permalloy film with its thickness of 25 nm. The signal input, pump wave input, and signal output are simple microstrip lines, thus the device structure is simple.

Quantitative characterization of a thin ferromagnetic film by pi-MFM and FMRM: Y. OUKHOV, I.H. LEE, D.V. PELEKHOV, Ohio State University, E. NAZARETSKI, Los Alamos National Lab, P. BANERJEE, P.C. HAMME, Ohio State University — We present a theoretical analysis of two new methods for high resolution magnetic characterization of magnetic materials. These two, probe-induced (pi) Magnetic Force Microscopy and Ferromagnetic Resonance Force Microscopy are related in exploiting the modification of sample properties by the magnetic field of the probe to enable new imaging capabilities. Our analytic theory enables quantitative modeling of signals obtained in these two microcopy methods, and so allows us to extract parameters describing the magnetic properties of ferromagnetic films. We compare our theory with experimental data and find excellent agreement. More detailed experimental data will be presented in an accompanying talk. Our methodology allows detailed local characterization of ferromagnetic films in complementary MFM and MRFM experiments.

This work was supported by US Department of Energy through the Grant No DE-FG02-03ER46054.

Thursday, March 19, 2009 2:30PM - 5:18PM – Session X30 DMP GMAG: Focus Session: Cobaltites 334

Doping fluctuation-driven magneto-electronic phase separation in La\(_{1-x}\)Sr\(_x\)CoO\(_3\) single crystals, CHRIS LEIGHTON, University of Minnesota — The doped perovskite cobaltites, in particular La\(_{1-x}\)Sr\(_x\)CoO\(_3\) (LSCO), have emerged as productive systems for the study of the magneto-electronic phase separation phenomenon widely observed in complex oxide materials. It is now well established that this system phase separates into hole-rich ferromagnetic clusters embedded in a hole-poor non-ferromagnetic insulating matrix at low doping. These clusters percolate at a critical doping value near \( x = 0.17 \) leading to a crossover from short- to long-range ferromagnetic order and a simultaneous insulator-metal transition. In this work we have used multiple complementary experimental probes (e.g. small-angle neutron scattering (SANS), heat capacity, and magnetotransport) to establish that high quality single crystals actually exhibit magnetic phase separation only over a well-defined doping range, 0.04 < \( x \) < 0.22. We further show that these limits can be perfectly reproduced by simple statistical simulations where the existence of local ferromagnetism is driven solely by the inevitable local compositional fluctuations that are present at such small length scales. These length scales are defined by the mean cluster size which is determined directly by SANS. The same simulations also reproduce the doping dependence of both the observed magnetic phase fractions and SANS intensity. A remarkable consequence of this analysis is that it suggests that the magnetic phase diagram measured on macroscopic specimens is applicable even at length scales as small as 1 nm. Most importantly, it is clear from this work that models based on true electronic phase separation are not required to explain the physical properties of these cobaltites. Co-authors: C. He, S. El-Khatib, J. Wu, (UMN), J.W. Lynn (NIST), H. Zheng, J.F. Mitchell (Argonne National Lab). Work supported by DoE and NSF.

Heat capacity study of magneto-electronic phase separation in La\(_{1-x}\)Sr\(_x\)CoO\(_3\) single crystals, C. HE, University of Minnesota, S. EISENBERG, C. JAN, University of Minnesota, H. ZHENG, J.F. MITCHELL, Argonne National Laboratory, J.W. LYNN, National Institute for Standards and Technology, C. LEIGHTON, University of Minnesota — We present an investigation of the specific heat (0.35 K < \( T \) < 270 K) and ordinary Hall effect (300 K) in La\(_{1-x}\)Sr\(_x\)CoO\(_3\) single crystals (0.00 < \( x \) < 0.30). The data reveal new information on the nature of the percolation transition, the crystal and electronic structure, and the magneto-electronic phase separation. The observations include a discontinuity in Debye temperature accompanying the percolation-type insulator-metal transition and a large electron mass enhancement, likely due to strong electron correlation effects. The various contributions to the heat capacity provide a detailed picture of the evolution of the phase-separated state with doping. Most importantly, this provides strong evidence for the anticipated result that the phase separation is restricted to a well-defined doping range, 0.04 < \( x \) < 0.22, in close agreement with recent small-angle neutron scattering.

Work supported by DoE and NSF.
Cobaltites, JUAN YU, DESPINA LOUCA, University of Virginia, DANIEL PHELAN, KEISUKE TOMIYASU, KAZUMASA HORIGANE, KAZUYOSHI YAMADA — The doping of holes into the non-magnetic Mott insulator, LaCoO$_3$, induces a magnetic inhomogeneous state resulting from competing magnetic phases. Elastic neutron scattering measurements on Ca, Sr, and Ba doped single crystals showed that phase competition is strongly dependent on the tolerance factor, $t$. When $t$ is small as in La$_{1-x}$Ca$_x$CoO$_3$, only a ferromagnetic (FM) phase is present. As $t$ gets large as in La$_{1-x}$Ba$_x$CoO$_3$, an incommensurate (IC) phase coexists with the FM phase. The IC phase becomes commensurate and as strong as the FM phase by $x \approx 0.18$, with a very long correlation length. This is in stark contrast to La$_{1-x}$Sr$_x$CoO$_3$, where the IC phase remains short-range and with its intensity reduced when the system orders ferromagnetically. Our observation shows that increasing $t$ enhances the presence of two phases and favors the growth of nanoscale spin-ordered superstructures. The subtle lattice changes brought about by changing $t$ have a direct effect on the Co-O hybridization that in turn affects the magnetic interactions. Double exchange interactions between Co$^{2+}$ and Co$^{4+}$ result in FM correlations while the superexchange between Co$^{2+}$ ions result in antiferromagnetic correlations giving rise to the second phase. This may be mediated by a Jahn-Teller mechanism that sets in at high temperatures.

Incommensurate charge and spin ordering in doped layered Co perovskite oxides: small-polaron charge glass, I. ZALIZNYAK, CMPMSD, Brookhaven National Laboratory, N. SAKIYAMA, ISSP, University of Tokyo, S.-H. LEE, University of Virginia, Y. MITSUI, H. YOSHIZAWA, ISSP, University of Tokyo — Using neutron diffraction, we have investigated two families of cobalt-based layered perovskite oxides, Pr$_2$-$_x$Ca$_x$CoO$_3$ ($0.39 < x < 0.73$) and La$_2$-$_x$Sr$_x$CoO$_3$ ($x = 0.5, 0.61$), which are relatives of high-Tc cuprate superconductors. In the range of heavy doping, $0.5 < x < 0.75$, we have discovered the doping-dependent incommensurate short-range ordering of charges and magnetic moments, whose scattering signatures look somewhat similar to those previously found in cuprates and nickelates. The average incommensurability of charge order (CO) propagation vector, $Q = (\epsilon_c, 0, 0)$, scales roughly linearly with doping and is proportional to the concentration of Co$^{2+}$ ions, $\epsilon_c \sim (1-x)$. CO exists already at room temperature and shows no change on cooling. In cobaltites, CO can be understood as a glassy state formed by nano-scale patches of commensurate small-polaron superlattices, whose average period is determined by the doping, $x$, but the long-range coherence is frustrated by the charge neutrality requirement. The magnetic spin order on cobaltites only develops at low $T < 40$ K. Its period is roughly twice that of CO, indicating dominant antiferromagnetic correlation between the nearest Co$^{2+}$ spins.

Core level line shape analysis of LaCoO$_3$, E. M. PAISLEY, J. STANLEY, J. HINTON, N. SUNDARAM, UC Santa Cruz, B. S. MUN, A. BOSTWICK, E. ROTENBERG, ALS, LBNL, J. F. MITCHELL, Argonne National Laboratory, D. P. BELANGER, G.-H. GWEON, UC Santa Cruz — The spin state of LaCoO$_3$ is a topic of high interest lately. Here we investigate the electronic structure of LaCoO$_3$ using core level and valence band photoemission spectroscopy. We compare the competing spin models in the literature by using our data obtained as a function of incident photon energy and temperature. Using line shape simulation of the Co 3s core level spectroscopy data and the Co 2p core level spectroscopy data, we address the issue of extracting the spin state information of the ground state from the photoemission data.

Incommensurate and commensurate charge and spin order in doped layered cobaltite oxides: small-polaron charge glass, I. ZALIZNYAK, CMPMSD, Brookhaven National Laboratory, N. SAKIYAMA, ISSP, University of Tokyo, S.-H. LEE, University of Virginia, Y. MITSUI, H. YOSHIZAWA, ISSP, University of Tokyo — Using neutron diffraction, we have investigated two families of cobalt-based layered perovskite oxides, Pr$_2$-$_x$Ca$_x$CoO$_3$ ($0.39 < x < 0.73$) and La$_2$-$_x$Sr$_x$CoO$_3$ ($x = 0.5, 0.61$), which are relatives of high-Tc cuprate superconductors. In the range of heavy doping, $0.5 < x < 0.75$, we have discovered the doping-dependent incommensurate short-range ordering of charges and magnetic moments, whose scattering signatures look somewhat similar to those previously found in cuprates and nickelates. The average incommensurability of charge order (CO) propagation vector, $Q = (\epsilon_c, 0, 0)$, scales roughly linearly with doping and is proportional to the concentration of Co$^{2+}$ ions, $\epsilon_c \sim (1-x)$. CO exists already at room temperature and shows no change on cooling. In cobaltites, CO can be understood as a glassy state formed by nano-scale patches of commensurate small-polaron superlattices, whose average period is determined by the doping, $x$, but the long-range coherence is frustrated by the charge neutrality requirement. The magnetic spin order on cobaltites only develops at low $T < 40$ K. Its period is roughly twice that of CO, indicating dominant antiferromagnetic correlation between the nearest Co$^{2+}$ spins.

Core level line shape analysis of LaCoO$_3$, E. M. PAISLEY, J. STANLEY, J. HINTON, N. SUNDARAM, UC Santa Cruz, B. S. MUN, A. BOSTWICK, E. ROTENBERG, ALS, LBNL, J. F. MITCHELL, Argonne National Laboratory, D. P. BELANGER, G.-H. GWEON, UC Santa Cruz — The spin state of LaCoO$_3$ is a topic of high interest lately. Here we investigate the electronic structure of LaCoO$_3$ using core level and valence band photoemission spectroscopy. We compare the competing spin models in the literature by using our data obtained as a function of incident photon energy and temperature. Using line shape simulation of the Co 3s core level spectroscopy data and the Co 2p core level spectroscopy data, we address the issue of extracting the spin state information of the ground state from the photoemission data.

Spin Glass Behavior in the new cobaltite series (BaSr)$_{1-x}$La$_x$CoO$_{15}$, OVIDIU GARLEA, RONGYING JIN, RADU C. STOICEA, Oak Ridge Natl. Lab., HAO SHA, Florida International University, JIANDI ZHANG, Florida International University and Louisiana State University — We report on the structural and magnetic properties of a new class of cobaltites with the chemical formula (BaSr)$_{1-x}$La$_x$CoO$_{15}$. These compounds crystallize in a hexagonal structure, where Co ions occupy two different sites with octahedral and tetrahedral oxygen environments. Four Co ions of the unit cell define the vertices of a tetrahedron and their mutual antiferromagnetic superexchange interactions are topologically frustrated. Partial substitution of Sr and Ba atoms for La allows one to adjust the degree of Co valence mixing and finely tune their magnetic interactions. A strong irreversibility between FC and ZFC magnetizations and the absence of magnetic reflections in the neutron diffraction patterns suggest a spin glass-like ground state for all the compositions.

Competition between Jahn-Teller instability and uniaxial magnetism in Ca$_2$CoMoO$_6$ (M = Mn, Co, Rh), YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, HONGJUN XIANG, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, ERJUN KAN, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, A. VILLESUZANNE, Institut de Chimie de la Matiere Condensee de Bordeaux (ICMCB-CNRS), Universite Bordeaux I, YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, A. VILLESUZANNE, Institut de Chimie de la Matiere Condensee de Bordeaux (ICMCB-CNRS), Universite Bordeaux I, YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, A. VILLESUZANNE, Institut de Chimie de la Matiere Condensee de Bordeaux (ICMCB-CNRS), Universite Bordeaux I, YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204.

Various magnetic ground states linked to sodium ordering pattern via controlled cooling in Na$_2$CoO$_2$ ($x \approx 0.75-0.85$), J. KANTER, W. WITTWER, T. SCHULZE, P. HAEFLIGER, S. PETTITJEAN, Laboratory for Solid State Physics, ETH Zurich, Switzerland, D. SHEPTYAKOV, CH. NIEDERMAYER, Laboratory for Neutron Scattering, PSI Villigen, Switzerland, K. MATTENCBERGER, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Detailed characterization is presented of a recently found link between the low temperature magnetic properties of Na$_2$CoO$_2$ and a sodium rearrangement process at the onset of sodium mobility around 200 K. Switching between different sodium ordering patterns is possible by adjusting the cooling speed, due to the long time constant of the sodium rearrangement. The various magnetic states (with $T_c$ of 6, 15 and 22 K) are characterized by transport, magnetization, specific heat and thermal expansion measurements and linked to the sodium ordering process. The magnetic field dependence of the transition temperatures and the magnetic anisotropy were studied in detail. Muon Spin Rotation experiments confirmed the true bulk character of the magnetic transitions and locally probed the different phases. Single crystal diffraction data links the different magnetic ground states to structural changes.
4:42PM X30.00010 A quantum Monte Carlo study of magnetism in the frustrated Hubbard model1, MATTHEW ENJALRAN, Department of Physics, Southern CT State University, New Haven, Connecticut — Motivated by the observation of complex phases in materials with quasi-two-dimensional triangular lattice structures, Na$_2$CoO$_2$ · yH$_2$O and κ-(ET)$_2$X, where nearest neighbor interactions are frustrated, we investigate the magnetic correlations in the 2D Hubbard model using constrained path quantum Monte Carlo. In order to develop our understanding of the effect of geometric frustration on the magnetic correlations in an itinerant electron model, we report results for the square and triangular lattice geometries at half-filling.

1Work supported by a Cottrell College Science Award, Research Corporation.

4:54PM X30.00011 Does disorder destroy e$_g$ pockets in Na$_{0.3}$CoO$_2$? A new ab initio method for disorder1, TOM BERLIN, DIMITRI VOLJA, WEI KU, Brookhaven National Laboratory/ Stony Brook University — Hydrated Na$_{0.3}$CoO$_2$ shows interesting superconductivity[1], with evidence of a nodal order parameter[2]. One possible origin of the nodal structure is f-wave pairing[3] due to the six e$_g$ pockets predicted by the local density approximation[4]. However, ARPES experiments[5] showed no sign of these hole pockets. In this talk, we will investigate a recent proposal[6] of destruction of the e$_g$ pockets due to disorder. An affordable ab initio Wannier function based method will be presented that takes into account spatial distributions of disorder, beyond existing mean-field approximations (e.g. VCA, CPA). We also use our Wannier functions to analyse the crystal field splitting, the sign of which critically determines the role of correlation in DMFT.

1Work partially supported by DOE-CMSN.

5:06PM X30.00012 Novel electronic states in the sodium rich phases of cobaltates Na$_x$CoO$_2$. MENG GAO, ZIQIANG WANG, Boston College — The cobaltates display many unusual properties in the sodium rich regime. We study the effects of strong local and finite range correlation and the sodium dopant order within the framework of an extended Hubbard model on the triangular lattice. We find that despite the proximity to the band insulating state at $x = 1$, the interplay of strong electronic correlation and sodium order leads to the formation of various unconventional inhomogeneous electronic states. We compare these findings to recent experimental observations around $x = 0.84$.

Thursday, March 19, 2009 2:30PM - 5:06PM –
Session X31 DMP GMAG: Focus Session: Magnetic Nanostructures: Domain Walls, Reversal, Oscillators 335

2:30PM X31.00001 Reversal mechanisms and defects in perpendicularly magnetized nanostructures. JUSTIN SHAW, NIST — The problem of switching field distributions (SFDs) is currently plaguing developing technologies which rely on uniform arrays of magnetic nanostructures such as bit patterned media, magnetic random access memory (MRAM) and spin-torque oscillators. Most of these technologies are shifting towards the use of perpendicularly magnetized materials due to the increased device performance and thermal stability that can be achieved. SFDs in such perpendicularly magnetized nanostructures can result from dot-to-dot interactions and size distribution, but is largely dominated by material defects [1- 4]. Such defects can arise from both the material deposition process, and post-deposition processing that occurs during nanofabrication. By comparing nanostructures fabricated by deposition on pre-patterned wafers to those fabricated by ion milling of continuous films, we show that the anisotropy of the edge region can be greatly different in each case. The size, temperature, and angular dependences of the reversal field indicate that the reversal mechanism also differs. In contrast to fabrication induced defects, microstructural variations manifest themselves as a random distribution of local anisotropies. We studied the anisotropy distribution in patterned elements by imaging the localized reversal of low anisotropy regions and mapping these sites as a function of applied field using MFM imaging and TEM. In addition, we used simulations to show the effect a small localized region of lower anisotropy material (such as a grain) has on the reversal field of the entire nanostructure. We find that the reversal field depends on both the relative anisotropy of the defect to the film, as well as, the location of the defect within the structure.


3:06PM X31.00002 Controlling Double Vortex States in Low-Dimensional Dipolar Systems, SERGEY PROSANDEEV, Research Assistant Professor, LAURENT BELLAICHE, 21-st century Professor in Nanotechnology, PHYSICS DEPARTMENT, UNIVERSITY OF ARKANSAS TEAM — The reversal process of the chirality of each opposite vortex belonging to a double vortex state in ferromagnetic hysterons, via the application of in-plane magnetic fields, is reported [1]. Simulations reveal that such a process involves the formation of four intermediate states, including original ones. Hysteresis loops can occur only in a counterclockwise fashion because of one of these intermediate states. Double vortex states can also be controlled by electric fields in ferroelectric nanostructures of different shapes, but with some key differences with respect to the ferromagnetic case.

3:18PM X31.00003 Magnetic domain wall shift registers for data storage applications, DAN READ, Imperial College London, L. O'BRIEN, H.T. ZENG, E.R. LEWIS, D. PETIT, J. SAMPAIO, L. THEVENARD, R.P. COWBURN — Data storage devices based on magnetic domain walls (DWs) propagating through permalloy (Py) nanowires have been proposed [Allwood et al. Science 309, 1688 (2005), S. S. Parkin, Imperial College London, L. O'BRIEN, H.T. ZENG, E.R. LEWIS, D. PETIT, J. SAMPAIO, L. THEVENARD, R.P. COWBURN — Data storage devices based on magnetic domain walls (DWs) propagating through permalloy (Py) nanowires have been proposed [Allwood et al. Science 309, 1688 (2005), S. S. Parkin, 3:42PM X31.00005 The boundary of the extended Hubbard model. MENG GAO, ZIQIANG WANG, Boston College — The cobaltates display many unusual properties in the sodium rich regime. We study the effects of strong local and finite range correlation and the sodium dopant order within the framework of an extended Hubbard model on the triangular lattice. We find that despite the proximity to the band insulating state at $x = 1$, the interplay of strong electronic correlation and sodium order leads to the formation of various unconventional inhomogeneous electronic states. We compare these findings to recent experimental observations around $x = 0.84$.

5:06PM X30.00012 Novel electronic states in the sodium rich phases of cobaltates Na$_x$CoO$_2$. MENG GAO, ZIQIANG WANG, Boston College — The cobaltates display many unusual properties in the sodium rich regime. We study the effects of strong local and finite range correlation and the sodium dopant order within the framework of an extended Hubbard model on the triangular lattice. We find that despite the proximity to the band insulating state at $x = 1$, the interplay of strong electronic correlation and sodium order leads to the formation of various unconventional inhomogeneous electronic states. We compare these findings to recent experimental observations around $x = 0.84$.

5:06PM X30.00012 Novel electronic states in the sodium rich phases of cobaltates Na$_x$CoO$_2$. MENG GAO, ZIQIANG WANG, Boston College — The cobaltates display many unusual properties in the sodium rich regime. We study the effects of strong local and finite range correlation and the sodium dopant order within the framework of an extended Hubbard model on the triangular lattice. We find that despite the proximity to the band insulating state at $x = 1$, the interplay of strong electronic correlation and sodium order leads to the formation of various unconventional inhomogeneous electronic states. We compare these findings to recent experimental observations around $x = 0.84$. 1Work supported by ONR grants N00014-04-1-0413 and N00014-08-1-0915, DOE grant DE-FG02-05ER46188 and NSF grants DMR-0701558, DMR-0404335 and DMR-0080054 (C-SPIN). Some computations were made possible thanks to the MRI Grants 0421099 and 0722625 from NSF. [1] S. Prosnadeev and L. Bellaiche, Physical Review Letters 101, 097203 (2008).

3:18PM X31.0003 Magnetic domain wall shift registers for data storage applications, DAN READ, Imperial College London, L. O'BRIEN, H.T. ZENG, E.R. LEWIS, D. PETIT, J. SAMPAIO, L. THEVENARD, R.P. COWBURN — Data storage devices based on magnetic domain walls (DWs) propagating through permalloy (Py) nanowires have been proposed [Allwood et al. Science 309, 1688 (2005), S. S. Parkin, Imperial College London, L. O'BRIEN, H.T. ZENG, E.R. LEWIS, D. PETIT, J. SAMPAIO, L. THEVENARD, R.P. COWBURN — Data storage devices based on magnetic domain walls (DWs) propagating through permalloy (Py) nanowires have been proposed [Allwood et al. Science 309, 1688 (2005), S. S. Parkin, 3:42PM X31.00005 The boundary of the extended Hubbard model. MENG GAO, ZIQIANG WANG, Boston College — The cobaltates display many unusual properties in the sodium rich regime. We study the effects of strong local and finite range correlation and the sodium dopant order within the framework of an extended Hubbard model on the triangular lattice. We find that despite the proximity to the band insulating state at $x = 1$, the interplay of strong electronic correlation and sodium order leads to the formation of various unconventional inhomogeneous electronic states. We compare these findings to recent experimental observations around $x = 0.84$. 1Work supported by ONR grants N00014-04-1-0413 and N00014-08-1-0915, DOE grant DE-FG02-05ER46188 and NSF grants DMR-0701558, DMR-0404335 and DMR-0080054 (C-SPIN). Some computations were made possible thanks to the MRI Grants 0421099 and 0722625 from NSF. [1] S. Prosnadeev and L. Bellaiche, Physical Review Letters 101, 097203 (2008).
3:30PM X31.00004 Ratchet Effects and Domain Wall Energy Landscapes in Amorphous Magnetic Films with 2D Arrays of Asymmetric Holes. J.I. MARTIN, A. ALLIA, I. SOBRADO, A. PEREZ-JUNQUERA, G. RODRIGUEZ-RODRIGUEZ, M. VELEZ, J.M. ALAMEDA, U. Oviedo-CINN, Oviedo, Spain, V.I. MARCONI, U. Nacional de Cordoba, Argentina, A.B. KOLTON, C. Atomico Bariloche, Argentina, J.M.R. PARRONDO, U. Complutense, Madrid, Spain — The driven motion of domain walls in extended magnetic films patterned with 2D arrays of asymmetric holes has been found to be subject to two different crossed ratchet effects [1] which results in an inversion of the sign of domain wall motion rectification as a function of the applied magnetic field. This effect can be understood in terms of the competition between drive, elasticity and asymmetric pinning as revealed by a simple model. In order to optimize the asymmetric hole design, the relevant energy landscapes for domain wall motion across the array of asymmetric holes have been calculated by micromagnetic simulations as a function of array geometrical characteristics. The effects of a transverse magnetic field on these two crossed ratchet effects will also be discussed in terms of the decrease in domain wall energy per unit area and of the modifications in the magnetostatic barriers for domain wall pinning at the asymmetric inclusions. Work supported by Spanish MICINN [1].

1 This work is supported by ONR MURI

3:42PM X31.00005 Magnetic Frustration in Nanowires: Domino Effect, SAMIR LOUNIS, PETER H. DEDERICHS, STEFAN BLÜGEL, Institut fur Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Julich, D-52425 Julich, Germany, STEFAN BLÜGEL TEAM. — The parity of the number of atoms in finite antiferromagnetic nanowires deposited on ferromagnetic substrates is shown to be crucial in predicting whether the magnetic ground state is non-collinear or collinear [1]. Using the full-potential Korringa-Kohn-Rostoker method for non-collinear magnetism [2] and a Heisenberg model we show that the magnetic structure of the whole nanowires dramatically changes if a single adatom is added. Infinite and finite nanochains with even number of adatoms are always magnetically non-collinear while odd number of atoms in the wire lead under given conditions to a collinear ferrimagnetic ground state. This unexpected nano-effect, which resembles a domino-effect, occurs only for wires at finite lengths. [1] S. Lounis, P. H. Dederichs, S. Blgel, Phys. Rev. Lett. 101, 107204 (2008). [2] S. Lounis, Ph. Mavropoulos, P. H. Dederichs, S. Blgel, Phys. Rev. B 72 224437 (2005).

3:54PM X31.00006 ABSTRACT WITHDRAWN

4:06PM X31.00007 Magnetic and mechanical characterizations of ultra-high frequency nano-electromechanical systems (NEMS). JOE LOSBY, N. LIU, Department of Physics, University of Alberta, C. HOLT, Department of Chemical and Materials Engineering, University of Alberta, D. MITLIN, Department of Chemical and Materials Engineering, University of Alberta and National Institute of Nanotechnology, A.E. FRASER, V. SAUER, W.K. HIEBERT, National Institute of Nanotechnology, M.R. FREEMAN, Department of Physics, University of Alberta and National Institute of Nanotechnology — Recent efforts in our group involve time-domain studies of the motion of silicon NEMS and spin dynamics in nanometer-scale permalloy elements. Transduction of microwave frequency (> 1 GHz) cantilevers, and time domain coherent control (“unringing”) of nanoscale resonators have been demonstrated. For the next stage of this work, we have fabricated permalloy NEMS cantilevers and doubly clamped beams in order to begin exploration of magnetomechanical dynamics in ferromagnetic nanostructures. The magnetization of these resonators is probed using time-resolved magneto-optical Kerr effect microscopy, while stroboscopic optical interferometry is used for the detection of vibrational modes. 1. N. Liu, F. Giesen, M. Belov, J. Losby, J. Moroz, A. E. Fraser, G. McKinnon, T. J. Clement, V. Sauer, W. K. Hiebert & M. R. Freeman, Nature Nanotechnology, In Press (2008). 2. Z. Liu, R.D. Sydora, and M.R. Freeman, Phys. Rev. B. 77. 174410 (2008).

4:18PM X31.00008 Synchronization of spin-torque oscillators via phase-shift control, JOHAN ÅKERMANN, Göteborg University and Royal Institute of Technology — The Spin Torque Oscillator (STO) shows great promise as a frequency generating device at microwave frequencies. However its very limited output power has to be significantly improved for any realistic application. One possibility is the synchronization of two or more STOs to both increase the microwave power and further increase Q. We have recently demonstrated an intrinsic preferred phase shift between an STO and an injected RF current [1, 2]. This phase shift has direct implications for current-mediated synchronization of serially connected STOs [3]. It is exactly at this phase shift where the multi-STO synchronized state develops the highest robustness and by tuning the total circuit I-V phase shift, synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]). More recently we have also found that the perpendicular torque synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]). More recently we have also found that the perpendicular torque synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]). More recently we have also found that the perpendicular torque synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]). More recently we have also found that the perpendicular torque synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]). More recently we have also found that the perpendicular torque synchronization can be enhanced by close to 2 orders of magnitude. Since our initial work, we have now determined both the phase shift and the enhancement factor in all types of STOs (standard, perpendicular [4], wavy torque [5], tilted polarizer [6]).

1 Supported by The Swedish Foundation for Strategic Research, The Swedish Research Council, The Göran Gustafsson Foundation, and the Knut and Alice Wallenberg Foundation. Johan Åkerman is a Royal Swedish Academy of Sciences Research Fellow.

4:54PM X31.00009 Microwave Emitting Nanomagnet Oscillator: Strongly coupled spin-photon modes, Ö.Ö. SOYKAL, M.E. FLATTE, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa — We describe a microwave emitting nanomagnet oscillator confined in a high Q-cavity. The precession of the magnetization of a typical Fe nanomagnet of 100 nm in radius, possessing roughly $10^{10}$ spins and described as a macrospin, is tuned to be in resonance with a microwave cavity of 1 mm in volume with an applied magnetic field. The Hamiltonian of the spin-cavity system is quantized in a fully quantum treatment. Due to the very large number of coherently-oriented spins, the interaction Hamiltonian of the spin-cavity system contains magnet-microwave mode coupling terms that exceed several GHz. Coherent coupling of the microwave field with nanomagnet spins is analyzed in terms of the coherent states of the spin-cavity system, which are characterized by large oscillations in the nanomagnet spin and cavity photon number, as well as by exceptionally long dephasing times. Therefore, the nanomagnet-cavity system is predicted to have distinguishable large total spin, long coherence times, and high power output. This may serve as an efficient means of transferring information between a magnetic and a photonic system.

1 This work is supported by ONR MURI
2:30PM X32.00001 A Spin-Orbital Singlet and Quantum Critical Point on the Diamond Lattice: FeSc$_2$S$_4$, GANG CHEN, UCSB, LEON BALENTS, ANDREAS SCHNEDER, Kavli Institute for Theoretical Physics, UCSB — We present a theory of spin and orbital physics in the A-site spinel compound FeSc$_2$S$_4$, which experimentally exhibits a broad “spin-orbital liquid” (SOS) regime. A spin-orbital Hamiltonian is derived from a combination of microscopic consideration and symmetry analysis. We demonstrate a keen competition between spin-orbit interactions, which favor formation of a local “Spin-Orbital Singlet”, and exchange, which favors magnetic and orbital ordering. Separating the SOS from the ordered state is a quantum critical point (QCP). We argue that FeSc$_2$S$_4$ is close to this QCP on the SOS side. The full phase diagram of the model includes a commensurate-incommensurate transition within the ordered phase. A variety of comparison to and suggestion for experiments are discussed.

2:42PM X32.00002 Quantum Critical Phenomena near Stoner Transition in Two Coupled Quantum Dots with Spin-Orbit Coupling, OLEKSANDR ZELYAK, GANPATHY MURTHY, University of Kentucky — We consider a system of two coupled quantum dots. Both the dots and connecting region are assumed to be in universal crossover regimes between Gaussian orthogonal and symplectic ensembles. Using a diagrammatic approach appropriate for energy separations much larger than the level spacing, we obtain the ensemble-averaged one- and two-particle Green’s functions. The diffusion and Cooperon parts of the two-particle Green’s function are described by separate scaling functions. We then use this information to investigate a model of interacting system in which one dot has Stoner exchange interaction, while the other is non-interacting but contains spin-orbit coupling.

3:06PM X32.00004 Cross-over of universality class in the Ising chain frustrated by long-range interactions, ALESSANDRO VINDIGNI, ETH Zurich, FABIO CINTI, University of Florence, OLIVER PORTMANN, DANilo PEScia, ETH Zurich — We investigate a spin chain in which the ferromagnetic nearest-neighbor exchange interaction $J$ competes with a long-range antiferromagnetic interaction of strength $g$ decaying spatially as $1/r^z$. For $\alpha$ smaller than a certain threshold $\bar{\alpha}$ (with $\bar{\alpha} > 2$), the long-range interaction is able to avoid the global phase separation — the uniformly magnetized state favored by the exchange interaction — even at $T = 0$. The ground state then consists of an ordered sequence of segments with equal length and alternating magnetization, resulting in a superlattice of magnetic domains. A memory of this periodic spin profile is retained at finite $T$ in the two-point correlation function, which oscillates as well but with a temperature-dependent period. Such an oscillation is then exponentially damped over a spatial scale, the correlation length, which diverges asymptotically, roughly, as the inverse of $T$. This suggests that the long-range interaction drives the Ising chain to acquire a universality class consistent with an underlying continuous symmetry. The $\epsilon T$-temperature dependence of the correlation length and the uniform ferromagnetic ground state, characteristic of the $g = 0$ discrete Ising symmetry, are recovered for $\alpha > \bar{\alpha}$.

3:18PM X32.00005 ABSTRACT WITHDRAWN

3:30PM X32.00006 Nature of topological quantum phase transition in chiral spin liquid, SUK BUM CHUNG, HONG YAO, Stanford University, EUN-AH KIM, Cornell University, STEVEN KIVELSON, Stanford University — How to best characterize and detect topological order, which is not associated with any local broken symmetry is one of central questions in the field of topological phases. While the ground state degeneracy that depends on the topology of the manifold the system is defined in has been a successful theoretical indicator of topological order, this concept is applicable only at $T = 0$ and not accessible experimentally. Another important indicator has been topological entanglement entropy. However, topological entanglement entropy at $T = 0$ can be the same for two distinct topological phases. Here we study an exactly solvable model first introduced in Ref.[1], motivated by the fact that the existence of topological quantum phase transition is known and the full spectrum is available. We examine the nature of Abelian to non-Abelian topological quantum phase transition by studying the expectation value of global flux which shows an abrupt jump at the critical point. We discuss the phase diagram of this quantum phase transition in terms of the global flux and entanglement entropy and discuss to what extent the existence of topologically ordered ground state with non-Abelian excitations is revealed at finite temperature. [1] H. Yao and S.A. Kivelson, PRL 99 247203 (2007).

3:42PM X32.00007 Scaling in modulated systems and reentrance of order, OLIVER PORTMANN, ALESSANDRO VINDIGNI, DANilo PEScia, ETH Zurich — Ultrathin ferromagnetic iron films exhibit a peculiar reentrance of order[1] A less symmetric pattern (stripes) that is present at lower temperatures reoccurs at higher temperatures after a more symmetric intermediate state (labyrinth). We obtain a good qualitative understanding of the system by analytically reducing this problem in two spatial dimensions to an effectively one-dimensional problem that retains important properties of the original system even in the presence of small deviations from mono-dimensionally modulated order. As revealed by a scaling analysis, this system is characterized by a highly anomalous temperature dependence of an elastic constant. This finding is corroborated by mean-field calculations. By means of the scaling analysis, we can relate this experimentally inaccessible elastic constant to experimentally measurable quantities. Comparison with experiment suggests that the driving force for the reentrance of order is indeed the strongly anomalous behavior of this elastic constant.

1 Supported by NSF DMR-0703992.

2 Orthorhombic SrRuO$_3$, JINGUANG CHENG, JIANSHI ZHOU, JOHN GOODENOUGH, TMI, University of Texas at Austin — SrRuO$_3$ is a metallic ferromagnet with $T_c \approx 160$ K where mean-field (MF) critical behavior has been observed. [1] Recently, we have shown that cubic BaRuO$_3$, which changes the bond angle $\angle$Ru-O-Ru changes the bond angle $\angle$Ru-O-Ru$_3$ versus $\sigma^2$, and introduces an A-cation size variance $\sigma^2$. The partial chemical substitution by either smaller Ca$^{2+}$ or larger Ba$^{2+}$ in Sr$_{1-x}$A$_x$RuO$_3$, which changes the bond angle $\angle$Ru-O-Ru$_3$ introduces an A-cation size variance $\sigma^2$, and $\langle r^2 \rangle$, causes a clear deviation from the MF behavior. In order to distinguish effects of $\angle$Ru-O-Ru versus $\sigma^2$, we have synthesized Sr$_{1-x}$Ca$_{0.5}$Ba$_{0.5}$RuO$_3$ under 1000°C and 10 GPa in a Walker-type multianvil; these samples have the same average $\angle$Ru-O-Ru$_3$, but a different $\sigma^2$. All samples exhibit perfect MF critical behaviors, which indicates that the peculiar bond angle $\angle$Ru-O-Ru$_3$ plays an essential role in determining the MF critical behavior of SrRuO$_3$.


3:54PM X32.00008 Generalized Onsager cavity field method for magnets with local spin fluctuations, JAMES GLASBRENNER, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, University of Nebraska - Lincoln — The Onsager cavity field method is extended to magnets described by a classical spin fluctuation model which interpolates between the limits of localized and itinerant magnetism and captures the qualitative features of itinerant thermodynamics. We find that both the interatomic exchange coupling and the on-site interaction are renormalized by short-range order. In the localized (Heisenberg) limit Onsager’s approximation is recovered, but in itinerant systems it is essential to include both corrections, for in this case a simple subtraction of only the Onsager reaction field leads to poor results. The generalized Onsager method is compared with the results obtained through mean-field and Monte Carlo methods. It is found that for close-packed lattices with nearest-neighbor exchange there is excellent agreement between the generalized Onsager method and Monte Carlo for any degree of itineracy, and offers a significant improvement over the mean-field approximation in predicting the Curie temperature [1]. [1] A. L. Wysocki, J. K. Glasbrenner, and K. D. Belashchenko, Phys. Rev. B 78, 184419 (2008)

4:06PM X32.00009 Spin Rotation Technique for Non-Collinear Magnetic Systems: Application to the Generalized Villain Model, J.T. HARALDSEN, R.S. FISHMAN, Oak Ridge National Laboratory — This work develops a new generalized technique for determining the static and dynamic properties of any non-collinear magnetic system. By rotating the spin operators in the local spin reference frame, we evaluate the zeroth, first, and second order terms in a Holstein-Primakoff expansion, and through a Green’s functions approach, we determine the structure factor intensities for the spin-wave frequencies. To demonstrate this technique, we examine the spin-wave dynamics of the generalized Villain model with a varying interchain interaction. The new interchain coupling expands the overall phase diagram with the realization of two separate spin configurations. The rotational Holstein-Primakoff expansion provides both analytical and numerical results for the spin dynamics and intensities of these phases. Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC.

4:18PM X32.00010 Edge States of Quantum Antiferromagnets, JOSÉ HOYOS, S. CHANDRASEKHARAN, H. U. BARANGER, Duke University — We investigate the edge states of spin systems in the Affleck-Kennedy-Lieb-Tasaki (AKLT) phase. Edges of correlated systems may show novel lower dimensional physics (as in quantum Hall edge states) and have recently garnered increasing experimental attention. Here we study spin-1 systems using the directed-loop quantum Monte Carlo technique. Depending on the configuration and parameters, even though the bulk system has a spin (Haldane) gap, the edge states can be gapless and described by an effective Luttinger liquid. We focus on the behavior of the edge states when the bulk undergoes a quantum phase transition from the AKLT to the Néel phase.

1Financial support: NSF

4:30PM X32.00011 Magnetic Properties of a Canted Antiferromagnet Mn(N₃)₂(4,4'-bpy), YOUCIF HAMIDA, DUSAN DANILOVIC, C.L. LIN, TAN YUEN, Dept. of Physics, Temple University, Philadelphia, PA, KUNHAO LI, JING LI, Dept. of Chemistry & Chemical Biology, Rutgers University, Piscataway, NJ — Results of magnetic susceptibility χ(T), isothermal magnetization M(H), and heat capacity C(T) measurements on a manganese complex with mixed ligands Mn(N₃)₂(4,4'-bpy) and Mn²⁺ moments, and a strong antiferromagnetic interaction of θ = 120 K. An antiferromagnetic transition with rather high transition temperature of 39 K was observed in the M(T)/H data of Mn(N₃)₂(4,4'-bpy), and large non-compensated component in χ(T) below T_N was seen. The result of M(H) measures showed that Mn(N₃)₂(4,4'-bpy) behaves like a ferrimagnet below T_N, with a small coercive field of H_c = 150 G at 1.8 K. A sizable anomaly was observed in C(T) data, and this confirms the long-range magnetic phase transition and the T_N. The magnetic behavior of this compound is discussed in terms of a strong Mn-Mn coupling through this unique network with end-to-end azido bridges, and compared with the magnetic behavior of its iron isostuctural analogue Fe(N₃)₂(4,4'-bpy).

4:42PM X32.00012 Magnetic switching and phase competition in the multi-ferroic antiferromagnet Mn₁₋ₓFeₓWO₄, FENG YE, Oak Ridge National Laboratory, Y. REN, Argonne National Laboratory, J.A. FERNANDEZ-BACA, H.A. MOOK, Oak Ridge National Laboratory, J.W. LYNN, NIST Center for Neutron Research, R.P. CHAUDHURY, Y.-Q. WANG, B. LORENZ, C.W. CHU, University of Houston — Elastic neutron scattering is used to study the spin correlations in the multiferroic Mn₁₋ₓFeₓWO₄ with x = 0.05, 0.05, and 0.10. The non-colinear incommensurate (ICM) magnetic structure associated with the ferroelectric (FE) phase in pure MnWO₄ is suppressed at x = 0.05 and completely absent at x = 0.10. The ICM spin order and FE phase can be restored by applying a magnetic field along the spin easy axis. The low-T° magnetic structure extends in both H/T with increasing Fe concentration. The systematic evolution of the magnetic and electric properties indicates that the noncollinear ICM spin order results from competing magnetic interactions and its stabilization can be tuned by the internal (x) or external magnetic-field perturbations.

3This work was partially supported by Division of Scientific User Facilities of the Office of Basic Energy Sciences, U.S. Department of Energy.

4:54PM X32.00013 The ferromagnetic transition in LiHoF₄, ANDERS BILTMO, PATRIK HENELIUS, KTH, Stockholm — The rare-earth magnetic compound LiHoF₄ is considered to be one of the best realizations of a long-range dipolar Ising model. Several experimental studies have been carried out probing the magnetic properties of the material in the context of classical, as well as quantum, phase transitions. In this work we revisit the effective model for the non-dilute material using numerical simulations. We examine the accuracy of the model in relation to experiments and consider the logarithmic corrections derived in renormalization group theory.

5:06PM X32.00014 Examination of the magnetic structure of Cs₂CuCl₄ by first principles DFT calculations, CHANGHOON LEE, Department of Chemistry, NCSU, JINHEE KANG, Department of Chemistry, Wonkwang University, S. Korea, MIKE WHANGBO, Department of Chemistry, NCSU — The spin-1/2 Cu²⁺ ions of Cs₂CuCl₄ have a 3D arrangement, but the magnetic properties of Cs₂CuCl₄ are mainly described by a quasi-2D triangular antiferromagnetic layer model. To understand why the 3D arrangement of (CuCl₄)²⁻ ions leads to a 2D magnetic behavior, we evaluated the various spin exchange interactions between adjacent (CuCl₄)²⁻ ions by performing DFT calculations. Our results show that the 6p orbitals of Cs⁺ participate in the spin exchange interaction through the Cl⁻Cs⁻Cl bridges if the two (CuCl₄)²⁻ ions have a symmetric arrangement and if the Cl⁻Cs⁻Cl bridges are symmetric, and that the frustrated 2D triangular antiferromagnetism originates from this selective participation of the Cs 6p orbitals in the spin exchange interactions.

1Professor Whangbo. thanks DMSE, OBES, and DOE
5:18PM X32.00015 Examination of the Coupled Magnetic-Structural Phase Transition in Gadolinium-Silicon-Germanium Magnetocaloric alloys at temperatures well above Tc. RAVI HADIMANI, EUGENE MELIKHOF, JOHN SNYDER, DAVID JILES, Wolfson Centre for Magnetics, Cardiff University, WOLFSON CENTRE FOR MAGNETICS TEAM — The first order phase transition in Gd5(Si2Ge1-x)14 from monoclinic phase to orthorhombic phase was investigated from 296-300 K at magnetic fields of up to 9 Tesla. The rate of change of transition temperature with magnetic field was found to be 4.9 K/Tesla in the field range up to 2.5 Tesla. This linear rate of change of transition temperature with field persisted even at higher magnetic fields of up to 9 Tesla. Measurements were made on single crystal Gd5Si2Ge1-x and Gd5Si2Ge2 using a high field VSM and a SQUID magnetometer. The single crystal samples were prepared by the Bridgman method at Ames Laboratory US DOE. The first order phase transition temperatures of single crystal samples at nearly zero field were determined to be 264 K and 267 K respectively. The magnetic field required to induce the first order phase transition at 289 K for the single crystal Gd5Si2Ge1-x was 4.8 Tesla and at 300 K it was 8 Tesla. For the single crystal Gd5Si2Ge2 sample, the magnetic field required to induce the first order transition at 289 K was 4.5 Tesla and at 300 K it was 8.4 Tesla. The magnetic field required to induce the first order phase transition increased linearly with the difference T-Tc.

This research is supported by the Royal Society under a Wolfson Research Merit Award.

Thursday, March 19, 2009 2:30PM - 5:06PM –
Session X33 DCMP: MgB2 and Multigap Superconductivity 403

2:30PM X33.00001 Homogeneity and connectivity of doped MgB2 bulks and strands as probed by heat capacity and transport current1, MIKE SUMPTON, MIKE SUSNER, MSE, The Ohio State University, Columbus, OH USA, Z. SHI, Department of Physics, Southeast University, China, E. COLLINGS, MSE, The Ohio State University, Columbus, OH USA — Homogeneity and current percolation have been investigated for MgB2 bulks and strands. Sintered bulks were compared to dense bulks produced by HIPping, infiltration, and spark plasma synthesis in terms of their homogeneity as measured by heat capacity and resistivity. Various levels of carbon based dopants were introduced in each case, with control samples for comparison. The influence of higher temperature processing on inhomogeneity was investigated. These results are compared to those of MgB2 based strands made both with and without C-based doping. In addition, comparisons of transport and magnetization measurements at higher magnetic fields showed the onset of a regime where the anisotropy between Jc parallel to the strand and Jc perpendicular to the strand grows rapidly. This leads to large differences between transport and magnetically measured values of not only critical current, but also the irreversibility fields. Birr. Such effects can be described in terms of three different regimes, defining the dimensionality of the system. These regimes are distinct from the various states of vortex matter present in the magnetic phase diagram of MgB2, but in coexisting with them they influence our estimates of these boundaries.

1This work was funded by the DOE HEP, Grant No. DE-FG02-95ER4, and by the Ministry of Education of the PRC, NECT, 0900.

2:42PM X33.00002 Upper critical field study of CH4 HPCVD carbon-doped MgB2, F. HUNTE, J. JAROSZYNSKI, A. GUREVICH, D.C. LARBALESTIER, NHMFL-Florida State University, Y. ZHU, P.M. VOYLES, University of Wisconsin, Madison, X.X. XI, K. CHEN, The Pennsylvania State University, S. BAILY, F. BALAKIREV, NHMFL-Los Alamos National Laboratory, C.G. ZHUANG, S. MENG, C.Y. ZHANG, Q.R. FENG, Z.Z. GAN, Peking University — The Hc2(T) of a set of four carbon-doped MgB2 films grown on both SiC and Al2O3 substrates by HPCVD from methane CH4 at flow rates from 7 to 10 sccm was measured in fields up to 65T. Compared to each metalorganic C sources which generated high Hc2(0), these films have much lower resistivities and higher connectivities. The curvature of Hc2(T) derived from low current four point magnetoresistance shows upturn at low temperatures, which is consistent with the dominance of π-band scattering in the theory of dirty two-gap superconductivity. Hc2(0) > 60 T is close to the paramagnetic limit of ~ 66 T for the 10 sccm film on SiC, though still a little lower than for the previously used metalorganic (Cu2H2)2Mg. Differences in the Hc2(T) behavior between films grown on the two substrates are attributed to variations in strain fields produced by the substrate coupled to the film at growth.

2:54PM X33.00003 Absolute Penetration Depth in MgB2, NICHOLAI SALOVICH, RUSSHEL GIANNETTA, Loomis Laboratory of Physics, Univ. of Illinois at Urbana-Champaign, Urbana IL 61801, MATT TILLMAN, PAUL CANFIELD, Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 — Absolute penetration depth measurements were carried out on single crystals of MgB2. λ(0) was determined by sputtering an Al film onto the sample crystal and measuring the change in Meissner screening as the Al film expels flux. The change in screening was measured with a tunnel diode oscillator [1]. Several samples were sputtered with films of different thicknesses and measured. Thickness dependent changes in Hc and Tc of the thin Al films provided a self-consistency check on properties of the films. Subsequent analysis using FIB/SEM and AFM independently measured the film thickness and roughness. Work at UIUC supported by NSF DMR-05-03982. Work at the Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358. [1] R. Prozorov, et al, Appl. Phys. Lett. 77, 4202 (2000)

3:06PM X33.00004 High Upper Critical Field and Critical Current Density of Carbon-doped MgB2 Films by HPCVD Using TMB, WENQING DAI, KE CHEN, QI LI, Department of Physics, Pennsylvania State University, University Park, PA 16802, XIAOXING XI, Department of Physics, Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA 16802 — Carbon-doping is effective to enhance upper critical field Hc2 and critical current density Jc of MgB2. Using Trimethylboron (TMB) as the doping source, we have successfully fabricated carbon-doped MgB2 thin films by the Hybrid Physical-Chemical Vapor Deposition (HPCVD) method. Large temperature derivative dHc2(0)/dT values near 4%, as high as 8.3 T/K, have been achieved for heavily doped samples. These values are much higher than what have been reported before. With Tc over 30 K, Hc2(0)/dT values over 100 T can be expected for these samples. For lightly doped films, Jc values, larger than 105 A/cm2 at 5 K under 9 T perpendicular field and 104 A/cm2 at 20 K under 5 T perpendicular field, were obtained. The results demonstrate that carbon-doped carbon-doped MgB2 films by HPCVD using TMB are promising for high field applications.

3:18PM X33.00005 Novel phase change in the mixed state of the multi-band MgB2 single crystal1, DAICHI KUBOTA, TAKEKAZU ISHIDA, Osaka Pref. Univ. (Sakai) — High-quality MgB2 single crystals of submillimeter size were synthesized successfully by the vapor transport method for carrying out magnetic torque measurements. The magnetic torque of MgB2 has been analyzed by a single-band model as well as a multi-band model for an anisotropic superconductor. The anisotropy in the coherence length 1/λ∥ and the anisotropy in the penetration depth 1/λ⊥ with the multi-band Kogan theory for the magnetic torque were simultaneously determined by means of the least-squares fittings. A systematic variation of two sorts of effective superconducting anisotropies, γ and λ, in the field-temperature plane was obtained as contours, and can be interpreted as a manifestation of the two-band nature of the MgB2 superconductivity. It is not a gradual crossover but a drastic change in the electronic state that an MgB2 superconductor transits from a π - σ multiband superconductor in lower fields to a σ single band superconductor in higher fields.

1This work was partly supported by a Grant-in-Aid for Scientific Research from the MEXT (Grant No. 19206104) and a special grant from Osaka Prefecture University.
Time Dependent Effects in Transport Measurements and Absence of Anisotropic Behavior in Polycrystalline MgB$_2$  

MURAT OLUTAS, ATILLA KILIC, KIVILCIM KILIC, ATILGAN ALTINKOK, HAKAN YETIS, KILIC TEAM — The flux dynamics in polycrystalline sample of MgB$_2$ have been studied by current-voltage (I-V) measurements for different sweep rates (dI/dt) of transport current at zero magnetic field (H=0) and H≠0, and also magnetovoltage measurements (V-H curves) for different sweep rates (dH/dt). It was observed that the time and hysteresis effects in I-V curves which appear upon cycling of transport current are not significant as compared to those of YBaCuO and BiSrCaCuO. The absence of hysteresis effects in I-V curves were attributed mainly to the absence of weak link structure in MgB$_2$. The hysteresis effects in V-H curves depend on field orientation of H with respect to I. Furthermore, it was observed that time dependent effects appear in V-H curves as the dH/dt varies and also the counterclockwise behavior which appears in forward region changes its character and becomes clockwise for reverse region. The magnetovoltage measurements were also carried out by varying the angle θ between H and I (V-θ curves). The V-θ curves show that there is no anisotropy in polycrystalline MgB$_2$. This behavior was discussed in terms of polycrystalline structure of MgB$_2$ and its band structure where the Fermi surface includes four sheets of one electron-like and three hole-like. The observations were interpreted mainly in terms of flux trapping in grains.

The conductivity percolation effects in CrO$_2$-MgB$_2$ nanocomposites  

XIANGDONG LIU, RAGHAVA PANGULURI, HUANG ZHI-FENG, BORIS NADGORYN, Department of Physics and Astronomy, Wayne State University, Detroit, MI 48201 — Cold-pressed half-metals/insulators are known to show an enhanced extrinsic powder magnetoresistance (MR) due to intergranular and intergrain spin-dependent tunneling. In this work we use a mixture of metal/superconductor (CrO$_2$)/(MgB$_2$)$_{1-x}$ nanocomposites to study conduction percolation effects. The samples were cold pressed in the form of pellets from the mixture of pure CrO$_2$ and MgB$_2$ powders. Transport and magneto-transport properties of various composition compacts measured as a function of temperature. Magneto-transport measurements performed over a temperature range of 2-100K show a hysteretic behavior with the peak values of MR coinciding with the CrO$_2$ coercive fields, with a maximum MR value for the composition near the percolation threshold of ∼ 42% at 2 K. The electrical resistivity displayed a sharp maximum near the percolation threshold, a feature that is likely to be unique for such systems of type. We will discuss the implications of our results for the analysis of conduction percolation within the framework of a simple percolation model and a possible connection to Andreev reflection effect in this system at low temperatures.

Flux penetration in mesoscale samples of multi-component unconventional superconductors  

DAVID GEORGE FERGUSON, PAUL GOLDBART, University of Illinois at Urbana-Champaign — Multi-component unconventional superconductors bring the possibility of unusual magnetic phenomena. Examples include spontaneous zero-field magnetization, and penetration by magnetic flux not only through one-dimensional vortices but also through two-dimensional domain walls in which superconductivity persists. How flux penetrates, both in and out of equilibrium, depends on the way in which the order parameter distorts—vortex versus domain wall—particularly in view of the fact that flux quantization is required for vortices but not for domain walls that traverse the sample. We study these issues in the setting of mesoscale samples, in which domain walls are more stable and any discreteness of flux penetration should be more readily observable, predicting an unusual variation of the magnetization with the applied magnetic field. The observation of such effects in Sr$_2$RuO$_4$, a proposed unconventional superconductor, via techniques such as cantilever torque magnetometry, should shed light on important issues such as the pairing symmetry and the prevalence of domain walls in bulk samples.
4:42PM X33.00012 Concomitant enhancement of spin susceptibility and pairing interaction in the reduced carrier-density regime of Li,ZrNCl superconductor . YUICHI KASAHARA, TSUKASA KISHIUME, TAKUMI TAKANO, KATSUKI KOBAYASHI, YOSHIHITO IWASA, IMR, Tohoku Univ., EIICHI MATSIUKA, HIDEYA ONODERA, Department of Physics, Tohoku Univ., YASUHIRO TAGUCHI, CMRG, ASI, RIKEN — Li-intercalated layered nitrides Li,ZrNCl are novel superconductors, in which superconductivity emerges at relatively high transition temperature \( T_c \sim 12 - 15 \) K with very low carrier density \( \sim 10^{21} \text{ cm}^{-3} \). The pristine \( \beta \) -ZrNCl is a simple band insulator, and electron doping is achieved by Li intercalation. Insulator-to-superconductor (IS) transition takes place at \( z \sim 0.05 \) with maximum \( T_c \) value of \( \sim 15 \) K and \( T_c \) decreases with further doping, which is opposite trend to the other superconductors in doped band insulators. Here we show the results of magnetic susceptibility measurements on Li\_2ZrNCl with systematically controlled \( z \). Estimated spin susceptibility \( \chi_s \) is almost temperature-independent without substantial anisotropy. With decreasing \( z \), \( \chi_s \) evolves strongly, same as \( T_c \). On the other hand, specific heat study revealed that the density of states is reduced but the pairing interaction is enhanced on the verge of IS transition. Therefore, our results may indicate that magnetic fluctuations are enhanced toward a band-insulator and that they are possibly responsible to superconductivity even in the present small carrier-density system.

4:54PM X33.00013 Absence of Superconductivity in the Hole Doped Li\(_{1+\delta}\)BC. ENGIN OZDAS, BORA KALKAN, EBRU GUNGOR, Advanced Materials Research Group, Physics Department, Hacettepe University, Beytepe, Ankara 06800, Turkey — The existence of several borocarbides with crystal structures highly related to MgB\(_2\), in which one of these, the layered LiBC has been predicted based on the electronic structure calculations that this compound should become superconducting on doping with holes. However, the superconducting features for Li off-stoichiometric borocarbid compounds have not been observed in any experimental studies, because of the difficulties in the sample preparation. In this work, the effects of synthesis conditions on the structure of Li\(_{1+\delta}\)BC samples with the different Li content and the phase stability were investigated. The structural studies showed that the intercalation process has a staging behavior as Li intercalated graphite and a novel Li vacancy ordered structure for off-stoichiometric stage-2 Li\(_{1+\delta}\)BC phase. The temperature dependence of the conductivity shows semiconducting behavior over the whole temperature range and the hopping type conduction improved by the hole doping.

Thursday, March 19, 2009 2:30PM - 5:30PM — Session X34 DCMP: Superconductivity: Magnetic Field Effects

4:24PM X34.00001 Ballistic acceleration phase of a supercurrent \(^1\) MILIND N. KUNCHUR, GABRIEL SARACLA \(^2\), University of South Carolina — One of the primitive but elusive current-voltage (I-V) responses of a superconductor is when its supercurrent grows steadily after a voltage is first applied, as per the first London equation. Because this phase lasts for a relatively short duration—until dissipative processes set in—it is difficult to conduct a correlated time-domain I-V measurement of it. The present work employed a measurement system that can simultaneously track and correlate I(t) and V(t) with sub-nanosecond timing accuracy, resulting in a clear time-domain measurement of this transient phase where the quantum system displays a Newtonian-like response. The highly controlled technique used here measures the near equilibrium response and should be distinguished from an impulse response measurement, which may probe non-equilibrium processes. The present technique should be valuable for the controlled investigation of other types of time-dependent and non-equilibrium phenomena.

4:24PM X34.00002 Spatial distribution of internal magnetic field in High T\(_c\) superconductors with pancake vortices. W.P. HALPERIN, S. MUKHOPADHYAY, A.M. MOUNCE, S. OH, Department of Physics and Astronomy, Northwestern University, IL, USA, A.P. REYES, P. KUHNS, National High Magnetic Field Laboratory, FL, USA, H. TAKAGI, Department of Physics, University of Tokyo, Tokyo, Japan, S. UCHIDA, Department of Advanced Materials Science, University of Tokyo, Chiba, Japan — We report here \(^{17}O\) \( T_1 \) measurements in single crystals of slightly overdoped \( (T_c = 82 \) K) Bi2212 at 5 K, in magnetic fields from 15 – 30 T. In previous work the internal magnetic field distribution in YBCO aligned powders at high magnetic fields has been probed by NMR imaging experiments [1]. Our results for single crystals of the highly anisotropic superconductor, BSCCO, are remarkably different, and is inconsistent with present theoretical predictions. At 5 K the system is in a 2-D vortex solid phase [2]. We conclude that the magnetic field distribution for 2-D vortices in the presence of interlayer magnetic and Josephson coupling is radically different from a London vortex lattice.

1This research was supported by the U. S. Department of Energy through grant number DE-FG02-99ER45763.

2Present affiliation: General Electric

2:54PM X34.00003 Intermittent propagation of magnetic flux in superconductors. \(^\ast\) VITALY YURCHENKO, ATLE JORSTAD QIVILLER, Iouri GALPERINE, University of Oslo, JOERN BINDSLEV HANSEN, PETER MOZHAEV, Technical University of Denmark, TOM HENNING JOHANSEN, University of Oslo, UNIVERSITY OF OSLO TEAM, TECHNICAL UNIVERSITY OF DENMARK TEAM — Regular arrays of planar defects can be introduced in superconducting YBa2Cu3O7 thin films by depositing them on tilted substrates. This results in anisotropy of critical currents flowing in the plane of the film. At optimal tilt angles a substantial increase of the critical currents flowing in both directions, i.e. along and across the planar defects, has been observed. However, the artificially introduced defects also have a dramatic effect on dynamics of the flux propagation: it becomes intermittent. Previously we observed intermittent flux penetration in MgB2 thin films with thermo-magnetic instability, where such flux jumps trigger giant magnetic avalanches. In this report we present results of a real time magneto-optical visualization of the intermittent flux motion in YBCO and discuss possible consequences for its thermo-magnetic stability.

3:06PM X34.00004 Magnetic field-orientation independence of large basal-plane critical currents in RBCO films with correlated pinning nanostructure \(^1\) DAVID CHRISTEN, Y.L. ZUEV, Oak Ridge National Laboratory, S.H. WEE, University of Tennessee, A. GOYAL, C. CANTONI, Oak Ridge National Laboratory, C. TARANTINI, A. GUREVICH, D. LARBALESTIER, Florida State University — It has been widely confirmed that self-assembled columnar stacks of second-phase precipitates aligned near to the c-axis provide strong pinning force in RBCO epitaxial films. Such growth-controlled nanostructures can be produced by at least two different deposition techniques and for several species of oxide precipitates. For many of these systems, the usual dependence of in-plane critical current densities, \( J_c \), on field-orientation nearly vanishes at a specific temperature-dependent field, \( B^\ast(T)\). The phenomenon can be described by a competition between intrinsic electronic anisotropy and orientation-dependent pinning. A simple model parameterizes the effect through the dependencies \( H_{irr}(\theta) \) and the power-law decay exponent \( \alpha(\theta) \), where \( J_c \propto H^{-\alpha(\theta)} \) in the intermediate field regime. Limits to and fundamental aspects of the model with respect to these parameters will be discussed.

1Research sponsored by the U.S. Department of Energy - Office of Electricity Delivery and Energy Reliability and by the Office of Science, Division of Materials Sciences and Engineering.
3:18PM X34.00005 Angularly Dependent, Contact-free Current Density Measurements of YBCO Coated Conductor, J.W. SINCLAIR, J.R. THOMPSON, Dept Physics, Univ. Tennessee, Knoxville, TN, USA, D.K. CHRISTEN, Y. ZHANG, Oak Ridge Nati Lab, Oak Ridge, TN, USA — Studying the angular dependence of the current density J gives insight into vortex pinning. We investigated a coated conductor of YBa$_2$Cu$_3$O$_{7-x}$ containing c-axis correlated defects (stacks of BaZrO$_3$ particles), striated into six strips to give a high aspect ratio. The current density was determined inductively from the magnetic moment $m \sim J$, using a SQUID magnetometer. The sample was mounted on a horizontal rotating platform to vary the angle $\Theta$ of the sample with respect to the vertical applied magnetic field. The magnetometer allows us to measure both the longitudinal and transverse components of moment $m(\Theta)$, enabling calculation of the angular dependence of $J$. For a large range of applied magnetic fields at various temperatures, we found a pronounced peak in $J(\Theta)$ at an angular value $\Theta_{peak}$ near the c-axis. We observed that, for a large range of applied magnetic fields, $\Theta_{peak}$ linearly scales with $1/h$, where $h = (H/H_{c2})$ is the reduced field. Research sponsored by DOE, Division of Materials Sciences and Engineering, and Office of Electricity Delivery and Energy Reliability.

3:30PM X34.00006 Vortex States in Intrinsic Josephson Junctions of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in High Parallel Magnetic Fields, JOVAN MIRKOVIC, Faculty of Sciences, University of Montenegro, G. Washington Str., 81000 Podgorica, Montenegro, SAITO TAKASHI, Institute of Materials Science, University of Tsukuba, 305-8573 Tsukuba, Japan, YUIMARU KUBO, National Institute of Materials Science, 2-1-2 Sengen, Tsukuba 305-0047, Japan, ITSUHIRO KAKEYA, Electronic Science and Eng. Faculty, University of Kyoto, 615-8510 Kyoto, Japan, AHMED ORAL, Faculty of Engineering and Natural Sciences, Sabanci University, Tuzla, 34956 Istanbul, Turkey, TAKASHI YAMAMOTO, KAZUO KADOWAKI, Institute of Materials Science, University of Tsukuba, 305-8573 Tsukuba, Japan — The $I_c$-axis resistivity measurements were performed in the vicinity of the ab-plane in order to investigate the interaction between Josephson vortices (JVs) and pancake vortices (PVs) in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ mesoscopic single crystals. It was found that the vortex lock-in transition becomes considerably broad in high magnetic fields, while the angular dependence of resistance exhibits the sharp lock-in features in low magnetic field region. The magnetic field dependence of the resistance exhibits the non-monotonic behavior probing the different vortex phases in tilted magnetic fields. Sharp dips and steps in the $c$-axis resistance were observed accompanied by penetration of quantized pancake vortices by tilting external fields from the ab-plane.

3:42PM X34.00007 Hole doping-induced evolution of self-organized bulk vortex structure in the high temperature YBa$_2$Cu$_3$O$_{7-\delta}$ superconductor, AHMAD MANSOUR, RONGCHAO MA, MEHMET EGLIMEZ, MURAT OLUTAS, HAKAN YETIS, KILIC TEAM — Time and hysteresis effects have been studied by magneto-transport measurements for high temperature YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) as a function of oxygen defect concentration $\delta$. These studies allowed us to map out the $(\mu,\delta)$ phase diagram of the vortex matter, where the exponent $\mu$ of the vortex structure was obtained using the scaling properties of the energy barrier against vortex motion. The reduction of the hole-doping level (an increase of $\delta$) of the material leads to a transformation of the vortex lattice into a glass and subsequently into a liquid phase. These vortex phases self-organize and produce relaxation plateaus in regions between step-like changes in the dependence of relaxation kinetics on hole doping, revealing the existence of a previously unknown correlation between the vortex structure and the hole-doping level in a cuprate superconductor, such as YBCO.

3:54PM X34.00008 Temperature Dependence of Flux Pinning Properties for Dilute Impurity Doped Y123 Single Crystals, YUI ISHI, Univ. Tokyo — Most of studies on pinning properties and relating vortex nature of the RE123 system were performed at high temperatures around 77 K, while extensive applications at low temperatures are also expected. However, both pinning properties and vortex states at low temperatures have not been well understood for RE123 crystals having intentionally introduced pinning sites. On the other hand, we have developed the chemical and versatile technique to introduce effective pinning site in the cuprates, that is dilute impurity doping for the target cation sites. In addition, compositional fluctuations of light rare earth (LRE) elements, which induce disorder transition of vortex system, are known to contribute enhanced pinning properties of LRE123. In this paper, we report that the changes of vortex state and $J_c$ characteristics of RE123 single crystals in $H//c$ at low temperatures by precise control of cation compositions. Our result suggested that dilute impurity doping to Cu (in CuO-chain) or Ba is more effective to enhance pinning strength of Y123 than introduction of compositional fluctuation for Gd123 single crystals at low temperatures below 70 K.

4:06PM X34.00009 Hysteresis Effects in Ag-Doped Superconducting Y-Ba-Cu-O, ATILGAN AL-TINKOK, KIVILCIM KILIC, ATILLA KILIC, MURAT OLUTAS, HAKAN YETIS, KILIC TEAM — Time and hysteresis effects have been studied by magnetovoltage $(V-H)$ curves measurements in Ag doped sample of YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO/Ag) as functions of transport current $(I)$, sweep rate of external magnetic field $(dH/dt)$ and temperature. Ag was added in the amount of 3% of nominal composition of Cu in YBCO. It was observed that the dissipation in V-H curves does not change as $dH/dt$ increases. This suggests that Ag doping destroys the weak-link structure along inter-grain boundaries and thus the vortices can find enough time to move in the sample irrespective of varying of external H. The hysteresis effects in V-H curves ride on a background voltage at the temperatures near the $T_c$. In one hand, the background voltage of V-H curves decreases by taking low values as the temperature decreases, in the other hand, the hysteresis effects become more significant. It was observed that the evolution of V-H curves depends also on the magnitude of transport current. The increase in $I$ causes a considerable enhancement in background voltage in V-H curves. Similar measurements were repeated for YBCO sample without Ag for a comparison. Experimental observations between YBCO/Ag and YBCO establish that adding of Ag into the superconducting matrix causes the formation of easy metallic flow paths for vortices and thus easy distribution of vortices along grain boundaries.

4:18PM X34.00010 Effect of pseudo-gap state to the vortices in the high-Tc cuprate superconductors, MASARU KATO, SATOSHI TOMITA, Osaka Prefecture University — The scanning tunneling spectroscopy (STS) experiments for high-Tc cuprate superconductor(SC) show the local density of states (LDOS) around a single vortex is different from that in a purely d-wave superconductor (dSC). Theoretically, in the dSC, there is a quasi-particle bound states peak around the vortex core, which is similar to that for an s-wave superconductor. This discrepancy means the superconductivity in high-Tc superconductors is simple dSC. In the high-Tc SC, dSC always coexists with unknown pseudo-gap state. Recent angle-resolved photoemission spectroscopy experiments show the energy gaps of pseudo-gap states and d-wave superconductivity are different. In this study, we show that the quasi-particle structure is reproducible theoretically, if we take into account the effect of the pseudo-gap state. We derived the Bogoliubov-de Gennes equation for the coexistence state with dSC and pseudo-gap (dSDW) state as the pseudo-gap state. We considered spin density wave (dSDW) state as the pseudo-gap state. We derived the Bogoliubov-de Gennes equation for the coexistence state with dSC and pseudo-gap state. We observed that, for a large range of applied magnetic fields, $\Theta_{peak}$ linearly scales with $1/h$, where $h = (H/H_{c2})$ is the reduced field. Research sponsored by DOE, Division of Materials Sciences and Engineering, and Office of Electricity Delivery and Energy Reliability.

3This work is supported by the FI program of Osaka Prefecture University.
4:30PM X34.00011 Magnetic field dependence of quasiparticle recombination times in superconducting NbTiN at low laser fluence. 

4:42PM X34.00012 Spin and charge dynamics of photogenerated quasiparticles in superconducting NbTiN.

4:54PM X34.00013 Quantum Oscillations from Fermi Arcs.

5:06PM X34.00014 Giant Thermomagnetic Effects in High-Tc Cuprates: Fermi Liquid vs Vortex Liquid.

5:18PM X34.00015 Absence of superfluid density anomaly at 0.6 K in superconducting PrOs\textsubscript{4}Sb\textsubscript{12}.

Thursday, March 19, 2009 2:30PM - 5:30PM –
Session X35 DMP: Focus Session: Iron Phnictides and Other Novel Superconductors XV: Electronic Structure and Magnetism

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2:30PM X35.00001 Electronic Structure of Fe-based Superconductors

DAVID J. SINGH, Oak Ridge National Laboratory — Understanding the electronic structure and electronic interactions in the layered Fe superconductors is prerequisite to understanding their superconductivity and other properties. The purpose of this talk is to overview results obtained within band structure approaches in relation to experiment. So far, many puzzles remain. The materials appear to be much more band-like and show much stronger signatures of metallic (Fermi surface related) physics than cuprates, with correspondingly weaker signatures of on-site Hubbard correlations. However, there remain substantial discrepancies between bare band structure calculations and experiment, and interestingly these discrepancies are in the opposite direction from those found in cuprates. These are discussed in the context of spin-fluctuations. This work was done in collaboration with I.I. Mazin, M.H. Du, Lijun Zhang, Alaska Subedi and Michelle Johannes.

1Work supported by DOE - Division of Materials Sciences and Engineering

3:06PM X35.00002 ABSTRACT WITHDRAWN —

3:18PM X35.00003 Theory for lattice collapse and frustrated magnetism in FeAs superconductors

RAFAEL FERNANDES, JOERG SCHMALIAN, Ames Laboratory and Department of Physics and Astronomy, Iowa State University — We present a theory for the pressure and temperature dependence of the magnetic and structural phase transitions in FeAs superconductors. Magnetic frustration in the FeAs planes leads to an enhanced coupling between lattice and magnetic degrees of freedom and is responsible for the strength of the first order transition from a paramagnetic tetragonal to an antiferromagnetic, orthorhombic phase. We analyze the phase diagram using a large N expansion for the magnetic degrees of freedom coupled to the lattice. Furthermore, we also address the importance of the lattice collapse in the CaFe2As2 compound and compare our predictions with experiments. Our results demonstrate that it is crucial to simultaneously include lattice and magnetic degrees of freedom for the FeAs systems.

3:30PM X35.00004 Formation and suppression of Fe magnetism in ferropnictides

IGOR MAZIN, MICHELLE JOHANNES, Naval Research Laboratory — First, I will address the issue of how the Fe magnetic moment in HTc pnictides is formed in the DFT calculation, why is it so large (up to 2 μB) and why the moments prefer to order in a stripe-like AFM manner. The role of the onsite Hund rule coupling in forming the moment and the role of one-electron (band) energy in selecting an AFM pattern will be explained and emphasized. The important distinction between AFM interactions local in real space (supercorrelation, e.g. in cuprates) and local in momentum space (SDW or AFM in ferropnictides, which is not an SDW in spin-Peierls sense). This part will be largely based upon our preceding talk. Next, I will present some speculations about possible solitonic fluctuations (dynamic AFM domain boundaries) in this system, and their relations to experiments. This pictures assumes that in the orthorhombic but nonmagnetic state the system consists of dynamic antiphase AFM domains, in the AFM state the domains are frozen (pinned), and in the nonmagnetic state dynamic twin domains dominate. This picture reconciles theory, thory and first principle calculations in surprisingly many aspects.

3:42PM X35.00005 First principles study of magnetic interactions and electronic structure in iron chalcogenide superconductors

MYUNG JOON HAN, SERGEY Y. SAVRASOV, University of California, Davis — By using first-principles density functional theory combined with linear response theory we investigate the magnetic interaction of the Fe chalcogenide high Tc superconductors, FeSe1-xTex. The exchange interaction terms are found to be different from those in pnictides, which suggests possibly different superconducting properties. The nearest neighbor antiferromagnetic coupling (J1a) is much stronger than the nearest neighbor ferromagnetic (J1b) and the next nearest neighbor coupling (J2). The J1a and J2 gradually decreases as x increases while J1b increases and becomes to be stronger than J2. Total energy calculation results and the electronic structure will be presented and compared to recent experiments.

3:54PM X35.00006 Microscopic origin of the structural and magnetic transitions in ferropnictide superconductor parent compounds

MICHELLE JOHANNES, IGOR MAZIN, DEVINA PILLAY, Naval Research Laboratory — The parent ferropnictide compounds exhibit two transitions: one is an orthorhombic distortion and the other is a magnetic transition. The transitions are simultaneous in the 122 structural type, but the structural transition precedes the magnetic one in the 1111 type. Although this temperature separation implies that the magnetism depends on the distortion, our computational results show that exactly the opposite is true. The structural distortion is fully dependent on the existence of magnetism and will not occur if a magnetic moment is not present. The particularities of the distortion, namely the expansion along the axis containing aligned spins, occurs as a result of minimizing the one-electron (band) energies. We show that the distortion depends not only on the existence of a magnetic moment, but on the particular ordering pattern chosen by the spins. Imposing a checkerboard ordering results in full x/y symmetry, while a so-called stripe ordering results in near perfect agreement with experimental neutron data below the transition temperature. Our results indicate that, even in the doped (superconducting) compounds, the underlying physics is magnetic.

4:06PM X35.00007 Magnetic Fluctuation and Anisotropy in High-Tc Iron Pnictides

QUAN YIN, MYUNG JOON HAN, WARREN E. PICKETT, SERGEY Y. SAVRASOV, University of California, Davis — Using first-principle density functional theory calculations combined with tight-binding method, dynamical mean field theory, and linear response theory, we extensively investigated the electronic structures and magnetic interactions of nine ferropnictides representing three different structural classes. The calculated magnetic interactions are found to be short-range, and the nearest (J1a) and next-nearest (J2) exchange constants follow the universal trend of J1a/2J2 → 1, despite their extreme sensitivity to the z-position of As. This suggests magnetic frustration as the key factor in stabilizing the superconducting ground state. The calculated spin wave dispersions show strong magnetic anisotropy in the Fe plane, in contrast to cuprates.

4:18PM X35.00008 Role of covalent Fe-As bonding in the magnetic moment formation and exchange mechanisms in iron-pnictide superconductors

KIRILL BELASHCHENKO, University of Nebraska-Lincoln, VLADIMIR ANTRPOV, Ames Laboratory — The electronic origin of the huge magnetoostructural effect in layered Fe-As compounds is elucidated using LiFeAs as a prototye. The crucial feature of these materials is the strong covalent bonding between Fe and As, which tends to suppress the exchange splitting. The bonding-antibonding splitting is very sensitive to the distance between Fe and As nuclei. We argue that the fragile interplay between bonding and magnetism is universal for this family of compounds. The exchange interaction is analyzed in real space, along with its correlation with covalency and doping. The range of interaction and itinerarity increase as the Fe-As distance is decreased. Supercorrelation makes a large antiferromagnetic contribution to the nearest-neighbor coupling, which develops large anisotropy when the local moment is not too small. This anisotropy is very sensitive to doping.
4:30PM X35.00009 The magnetic interactions in iron pnictides, JUJU PULIKKOTIL, VLADIMIR ANTROPOV, Ames Laboratory, Ames, I, USA, MARK VAN SCHILFGAARDE, Arizona State University, Tempe, AZ, USA — Using static linear response theory we studied the pair wise magnetic interaction parameters in many typical families of iron pnictides. Parameters have been obtained for a wide range of volumes and distance between Fe and As atoms. We demonstrate that two nearest neighbor couplings in plane dominate, with a third and fourth nearest neighbor coupling responsible for the appearance of non-collinear ordering when the magnetic moment is small. We found that the ratio between first and a second neighbor coupling is not universal and greatly varies as a function of pressure or Fe-As distance. A small interplane coupling is found, and it varies by a factor of 10-20 among pnictides. We analyze the Neel temperatures, adiabatic spin wave spectrum and a nature of magneto-structural transitions in different classes of pnictides.

4:42PM X35.00010 The magnetic phase diagram of iron pnictides, GERMAN SAMOLYUK, JUJU PULIKKOTIL, VLADIMIR ANTROPOV, Ames Laboratory, Ames, IA, 50011 — We study the stability of magnetic structures in iron pnictides as a function of doping, external pressure and the amount of defects. Several collinear and non-collinear magnetic structures are found to be stable in all classes of pnictides. This stability however is a result of a fragile competition between several nearest neighbor exchange couplings and depends greatly on doping. We determined that for a relatively small electron doping the non-magnetic instability is developed, while already for a small hole doping the stripe structure is instable in many pnictides and other magnetic structures are stabilized. For a larger hole doping the local magnetic moment phase with ferromagnetic long range order can be stabilized. A transition to non-collinear state at small moments is explained by a competition between the anisotropy of the nearest neighbors exchange couplings and third or forth neighbor couplings. Using very extensive calculations of magnetic stability parameter we build a generic pressure-concentration phase diagram of iron pnictides.

4:54PM X35.00011 Magnetic excitations in iron pnictides, VLADIMIR ANTROPOV, Ames Laboratory, Ames, IA, USA, LIQIN KE, TAKAO KOTANI, MARK VAN SCHILFGAARDE, Arizona State University, Tempe, AZ, USA — We analyze the dynamical spin susceptibility \( \chi(q, \omega) \) in the iron pnictides: FeSe, CaFe2As2 and SrFe2As2 and obtain the spectra of spin excitations. In the long wavelength limit we obtain parameters for the effective Heisenberg model and compare it with parameters generated by a static response method. Antiferromagnons are found for a small \( q \), while for the larger \( q \) strong Stoner excitations are developed. These results support the claim that iron pnictides are marginally itinerant systems. We also estimate zero-point fluctuations from \( \chi \) and find the following contributing mechanisms: adiabatic spin waves, hole-particle Stoner excitations and longitudinal fluctuations. Taking these effects into account improves the agreement between theory and experiment and indicate the importance of itinerant spin fluctuations.

5:06PM X35.00012 Collinear (Bi-collinear) antiferromagnetic order in iron-pnictides (chalcogenides)\(^1\), ZHONG-YI LU, Department of Physics, Renmin University of China, Beijing 100872, China, FENGJIE MA, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China, TAO XUAN, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — By the first-principles electronic structure calculations, we find that the ground state of the tetragonal \( \alpha \)-FeTe is in a bi-collinear antiferromagnetic order, in which the Fe local moments (~ 2.5\( \mu_B \)) align ferromagnetically along a diagonal direction and antiferromagnetically along the other diagonal direction on the Fe–Fe square lattice. This novel bi-collinear order results from the interplay among the nearest, the next nearest, and the next next nearest neighbor superexchange interactions, mediated by Te 5p-band. In contrast, the ground state of the iron pnictides or chalcogenides is in a conventional collinear antiferromagnetic order, like LaFeAsO, resulting from the interplay between the nearest and the next-nearest neighbor superexchange antiferromagnetic interactions, bridged by As atoms. This finding sheds new light on the origin of magnetic ordering in Fe-based superconductors.

\(^1\)This work is partially supported by National Natural Science Foundation of China and by National Program for Basic Research of MOST, China.

5:18PM X35.00013 Effective Hamiltonian for FeAs based superconductors\(^1\), EFRATIATOS MANOUSAKIS, Department of Physics and MARTECH, Florida State University, Tallahassee, Florida, 32306, USA and Department of Physics, University of Athens, Greece — The Fe-pnictide superconductors exhibit unusual properties attributed to electrons and holes occupying the Fe \( d \)-orbitals and the outermost occupied \( s \) and \( p \) pnictide orbitals. Starting from the atomic limit, we carry out a strong coupling expansion for the FeAs layer, where the on-site Coulomb repulsion parameters are assumed to be significantly larger than the hopping between Fe \( d \) orbitals and the hybridization parameters between the Fe \( d \) and As \( 1s \) or \( 1p \) orbitals; we derive an effective Hamiltonian that describes the low energy electron/hole behavior. If this condition for strong coupling expansion is not satisfied, still, we believe that our qualitative results capture important aspects of the physics in these materials. The hopping and the hybridization parameters are obtained by fitting the results of our calculations based on the local density approximation to a tight-binding model. The effective Hamiltonian, in the strong coupling limit, consists of three parts which operate on the three subspaces coupled through Hund’s rule and spanned by the following Fe orbitals: (a) the \( d_{x^2-y^2} \); (b) the degenerate orbitals \( d_{xz} \) and \( d_{yz} \); and (c) the \( d_{xy} \) and \( d_{z^2} \). Each of these parts is an extended \( t'-t'' \rightarrow J'-J'' \) model and is characterized by different coupling constants and filling factors. For the undoped material the second subspace alone prefers a ground state characterized by a spin-density-wave order similar to that observed in recent experimental studies, while the other two subspace prefer \( (\pi, \pi) \) antiferromagnetic order. The observed spin-density-wave order is imposed by the \( d_{z^2} \) subspace as the ground state of the total Hamiltonian of the undoped parent compounds. However, due to the above mentioned frustration the magnetic moment is small in agreement with observation. Our calculation illustrates in a simple manner the reason for the difference in the magnetic ordering between the Fe-pnictides and the cuprates. It also suggests a different evolution of the magnetic order upon electron versus hole doping.

\(^1\)In collaboration with J. Ren, S. Meng and E. Kaxiras, Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA. Phys. Rev. B 78, 205112 (2008)

Thursday, March 19, 2009 2:30PM - 5:06PM — Session X36 DCMP: Glassy, Amorphous, and Quasicrystalline Materials 408

2:30PM X36.00001 Using First-Principles Calculations to Describe Amorphous Metal Films for Hydrogen Purification, SHIQIANG HAO, MIKE WIDOM, DAVID SHOLL, GEORGIA INSTITUTE OF TECHNOLOGY TEAM, CARNEGIE MELLON UNIVERISTY TEAM — The increasing demand for clean and efficient energy has resulted in an increased global willingness to embrace the proposed hydrogen economy. The use of amorphous metal films as membranes to purify hydrogen has potential to overcome at least some of the disadvantages of existing crystalline metal membranes. We introduce a general strategy combining density functional theory and statistical mechanics to quantitatively predict solubility, diffusivity and permeability of interstitial \( H \) in amorphous metals. Our methods make it possible for the first time to quantitatively evaluate the performance of amorphous metal films as hydrogen purification membranes. These methods are introduced by examining amorphous Fe3B and a crystalline analogue with the same composition. A membrane made from the amorphous material is predicted to have a hydrogen permeability 1.5-2 orders of magnitude higher than a crystalline membrane. The methods we introduce here will be useful in accelerating the development of amorphous membranes for practical applications.
Can be improved by partially replacing elements such as boron and carbon that create ionic and covalent bonds with other elements such as phosphorous that do not contain phosphorus, and the Poisson’s ratios obtained are correspondingly high. The ductility of amorphous steels can be improved by chemically tuning the increased with the decrease in shear modulus. The shear moduli are appreciably lower than those reported for previous amorphous steel compositions that did not contain phosphorus, and the Poisson’s ratios obtained are correspondingly high. The ductility of amorphous steels can be improved by chemically tuning the elastic properties which are determined by the amorphous structure and chemical bonding. First-principles electronic structure calculations show that ductility can be improved by partially replacing elements such as boron and carbon that create ionic and covalent bonds with other elements such as phosphorous that favor metallic cohesion.

1Supported by the DARPA Structural Amorphous Metals Program under ONR Grant No. N00014-06-1-0492

2:42PM X36.00002 Atomic structure of PdNiP bulk metallic glass from ab initio simulations. VIJAY KUMAR, Dr. Vijay Kumar Foundation, Gurgaon, India; T. FUJITA, M.W. CHEN, WPI-AIMR, Tohoku Univ. Sendai, Japan; A. INOUE, Tohoku Univ., Sendai, Japan; Y. KAWAZOE, IMR, Tohoku Univ. Sendai, Japan — The atomic structure of Pd40Ni40P20 bulk metallic glass (BMG) has been simulated using ab initio molecular dynamics plane wave method and PAW pseudopotentials. We use generalized gradient approximation to calculate the exchange-correlation energy and a cubic simulation box whose size and shape have been optimized after the BMG has been formed in simulations. The resulting radial distribution function and density agree remarkably well with the experimental data. The structure is analysed in terms of local clusters centered around Pd, Ni and P atoms and their electronic structures have been used to understand the bonding, stability, and the formation of the PdNiP BMG.

2:54PM X36.00003 Role of Electronic Structure on Ductility of Iron-Based Bulk Metallic Glasses1, N. KVALTINE, X.J. GU, S.J. POON, G.J. SHIFLET, University of Virginia, M. WIDOM, Carnegie Mellon University — Composition effects on the mechanical properties of iron-based amorphous steel alloys have been investigated, with attention to the metalloid content and the relative impact of boron, carbon and phosphorous. Phosphorous-containing amorphous steels exhibited enhanced plastic strains and fracture strengths. Moreover, the plastic strain increased with the decrease in shear modulus. The shear moduli are appreciably lower than those reported for previous amorphous steel compositions that did not contain phosphorus, and the Poisson’s ratios obtained are correspondingly high. The ductility of amorphous steels can be improved by chemically tuning the elastic properties which are determined by the amorphous structure and chemical bonding. First-principles electronic structure calculations show that ductility can be improved by partially replacing elements such as boron and carbon that create ionic and covalent bonds with other elements such as phosphorous that favor metallic cohesion.

1Supported by the DARPA Structural Amorphous Metals Program under ONR Grant No. N00014-06-1-0492

3:06PM X36.00004 Bond enthropy trends of high metalloid Fe-based bulk metallic glasses, M. WIDOM, B. SAUERWINE, Carnegie Mellon University, N. KVALTINE, X.J. GU, S.J. POON, G.J. SHIFLET, University of Virginia — Chemical bond types in metal-metalloid glass-forming compounds range from metallic to ioniic and covalent. Iron-rich alloys are dominated by metallic bonding, but charge transfer from iron atoms to highly electronegative metalloid elements such as boron, carbon and phosphorous creates ionicity, and the metalloid bonding is intrinsically covalent. For sufficiently large metalloid content their strong bonding character must increase the shear modulus, leading to an associated increase in brittleness of the material. However, for metalloid fractions below 30%, shear modulus is found to decrease with increasing metalloid content, leading to an associated increase in ductility of the material. We show this unexpected decrease in shear modulus is caused by depletion of the charge density around the iron atoms, weakening the iron-iron bonds. Our calculations are based on Crystal Orbital Hamilton Populations (COHPs) for crystalline structures that locally approximate the amorphous structure.

3:18PM X36.00005 Effect of excess electrons on hexagonal close-packed Mg and the model clusters for bulk metallic glasses, MASAE TAKAHASHI, MIKIO FUKUHARA, AKIHISA INOUE, YOSHIYUKI KAWAZOE, Tohoku University — Though empirical rules for a large glass forming ability (GFA) were proposed, the formation mechanism of the bulk metallic glasses (BMGs) and the main factors for the GFA have not been clearly elucidated. The advantages of Mg-based BMGs are the lightness and abundance of resources, and a wide supercooled liquid region with the very high thermal stability and extremely large GFA. In 1991, Inoue et al developed glassy Mg–Cu–Y alloys with a maximum diameter of 4.0mm. We report here the effect of excess electrons on hexagonal close-packed Mg and the model clusters explained by an inflation process using density functional theory-based calculations, in order to understand the role of conduction electron concentration (CEC) in Mg-based BMGs [M. Takahashi et al., J. Phys. D: Appl. Phys. 2008, 41, 155424]. The CEC of Mg increase in Mg-based BMGs. In our model calculations, the increased CEC is artificially realized by the injection of electrons into Mg clusters and hcp Mg. We find the volume expansion and distortion to a higher c/a ratio in the negative charge state. The increase in the values corresponding to the c/a ratio is also observed in the model clusters. In the density of states at the equilibrium cell parameters expanded by charging, the pseudogap near the Fermi level by α–π mixing becomes small and a spiky structure appears.

3:30PM X36.00006 Toward Understanding the Giant Frictional Anisotropy on AlNiCo. KEITH MCLAUGHLIN, HEATHER HARPER, DAVID RABSON, University of South Florida — In a 2005 article in Science [309, 1354], Park et al. measured in vacuum the friction between a coated atomic-force-microscope tip and the clean two-fold surface of an AlNiCo quasicrystal. Because the two-fold surface is periodic in one direction and aperiodic (with a quasiperiodicity related to the Fibonacci sequence) in the perpendicular direction, frictional anisotropy is not unexpected; however, the magnitude of that anisotropy in the Park experiment, a factor of 8, is unprecedented. By eliminating chemistry as a variable, the experiment also demonstrated that the low friction of quasicrystals must be tied in some way to their quasiperiodicity. Through molecular-dynamics simulations with pair potentials on quasiperiodic approximants, we investigate generic geometric mechanisms that might give rise to this anisotropy.

3:42PM X36.00007 Does the morphology of fracture surfaces reveal the structure of quasicrystals? LUC BARBIER, DANIEL BONAMY, CEA, Saclay, France; LAURENT PONSON, California Institute of Technology, Pasadena, USA — The roughness of surfaces obtained by cleavage of l-AlPdMn quasicrystals at room temperature are analyzed using tools of quantitative fractography. From the atomic scale up to 3 nm, they are shown to exhibit scale invariance properties hiding the cluster (0.45 nm) aperiodic structure. These properties are quantitatively similar to those observed on various disordered materials, albeit on other ranges of length scales. These properties are interpreted as the signature of damage mechanisms occurring within a 3 nm wide zone at the crack tip. The size of this process zone finds its origin in the local temperature elevation at the crack tip. This effect is not expected to be responsible for a transition from a perfectly brittle behavior to a nanoductile one. It explains also why the cluster structure of quasicrystals is not revealed on the fracture surfaces of l-AlPdMn broken at room temperature.

3:54PM X36.00008 Quasicrystal Growth and Thermal Expansion, SALLY JUNE TRACY, JASON COOLEY, HEATHER VOLTZ, JASON LASHLEY, Los Alamos National Laboratory — We have grown Au-Mn-Pd and RE-Mg-Zn quasicrystals (RE=Y, Er, Ho, Dy and Tb) from a high temperature metallic solution using a self-flux method with melt compositions presented in previous work by Canfield and Fisher1 The samples showed dodecahedral grains with pentagonal facets. The icosahedral structure was revealed with x-ray powder diffraction. We were able to index the diffraction patterns using Cahn’s two index scheme2 We have measured the thermal expansion of these samples and will present this data.

1High temperature solution growth of intermetallic single crystals and quasicrystals; Canfield, P.C.; Fisher, I.R., Journal of Crystal Growth (May 2001) Vol. 255, is 2-4, p. 155-161
2Indexing of icosahedral quasiperiodic crystals; Cahn, J.W.; Shechtman, D.; Gratias, D., Journal of Materials Research (Jan.-Feb.) vol. 1, no. 1, p. 13-26
A surprising result is confirmed by both DFT and Configuration Interaction. That both structures must be present in the cluster beam, even in cases where the higher energy isomer is up to 0.5 eV higher than the ground state. This is due to the fact that the photoelectron spectrum of small NbC<sub>n</sub> clusters is variable effects of doping on the electronic structure depending on the precise geometry and electron count. 

We calculate the photoelectron spectrum of small NbC<sub>n</sub> clusters using Dynamical X-ray scattering [1]. Under field, anisotropic translational dynamics and aging are observed. Moreover, a strong anisotropic cooperativity is reported, almost hundred times larger in the parallel direction. The results are discussed using a phenomenological picture. [1] E. Wandersman et al., J. Phys. Cond. Mat. 20 (2007) 155104

Gradient interactions and the low temperature universality in glasses, MOSHE SCHECHTER, PHILIP STAMP, University of British Columbia — Amorphous solids show striking universal characteristics at low temperatures, including unique temperature dependencies of the specific heat, thermal conductivity and internal friction, and a small and rather constant ratio between a phonon wavelength and its mean free path. These universal phenomena are observed in polymers and disordered lattices as well. The standard tunneling model proposed by Anderson, Halperin and Varma, and Philips, accounts well for much of the observed phenomena. However, questions regarding the nature of the two-level systems, the smallness of the above ratio, and the energy scale dictating the temperature range of the phenomena, remain unanswered. We propose a theory that suggests an answer to these questions, along with an explanation of the additional observed phenomena connected with the universal behavior. Our theory is rigorously derived for disordered lattices, and we argue for the plausibility of its applicability to amorphous solids.

Moment based approach to electronic structure calculations: applications to ordered and disordered systems, HIRO SHIMOYAMA, The University of Southern Mississippi, PARTHAPRATIM BISWAS, University of Southern Mississippi — We solve the classical moment problem via maximum entropy optimization to calculate the electronic density of states for ordered and disordered solids. The method employs the Shannon entropy functional and maximize it subject to the moment constraints to construct the spectral distribution of large Hamiltonian-matrices. We illustrate the efficiency and usefulness of the method by applying three candidate systems: a crystalline semiconductor, an amorphous material; and a completely disordered system via tight-binding Anderson model Hamiltonian. The band energy and Fermi level are computed from the reconstructed density of states with a high degree of precision. A possible extension of this method to calculate electronic forces is also discussed.

What is a dynamical glass transition?, CLAUDIO CHAMON, Boston University, CLAUDIO CASTELNOVO, DAVID SHERRINGTON, University of Oxford — Using the mapping between the Fokker-Planck description of classical stochastic dynamics into a quantum Hamiltonian, we argue that a dynamical glass transition must have a precise definition in terms of a quantum phase transition. At the static level, the transition affects the ground state wavefunction: while in some cases it could be picked up by the expectation value of a local operator, in others the order may be non-local, and impossible to be determined with any local probe. In general, even in the absence of a local order parameter, the transition can be detected via the quantum fidelity of the groundstate wavefunction, which we show translates directly into a singularity in the heat capacity of the classical system. We illustrate these ideas using exact diagonalizations of the mapped Hamiltonians for the p-spin models and the gonihedric model.

Session X37 DCP: Spectroscopy and Dynamics of Single Molecules and Nanoparticles

Reactivity of Aluminum and Doped Aluminum Clusters, ARTHUR REBER, SHIV KHANNA, Virginia Commonwealth University, PATRICK ROACH, WILLIAM WOODWARD, A. WELFORD CASTLEMAN JR., Penn State University — We examine the reactivity of aluminum cluster anions with water, and other nucleophiles. The clusters reveal size dependent reactivity which primarily results in either the chemisorption of one or more water molecules, or no observable reactivity. The reactivity of the clusters is found to be dependent on surface sites which facilitate the splitting of the water on the surface of the cluster. Clusters with two sets of active sites are found to selectively release molecular Hydrogen. We also investigated the reactivity of aluminum clusters doped with another metal and their reactivity with molecular Oxygen. As the reactivity of aluminum clusters with oxygen depends on the electronic shell closing, this serves as a probe of the effects of doping on the electronic shell structure. The results reveal variable effects of doping on the electronic structure depending on the precise geometry and electron count.

Multiple Isomers in the Photoelectron Spectra of NbC<sub>n</sub> clusters, IVAN IORDANOV, JORGE SOFO, Department of Physics, Penn State — We calculate the photoelectron spectrum of small NbC<sub>n</sub> clusters (2<n<7), to identify the atomic structure that best matches experimental photoelectron spectra. We use Density Functional Theory calculations to find all stable isomers. In order to obtain more accurate spectra, we use the Symmetry Adaptor Cluster Configuration Interaction method for the smaller clusters where the highly correlated niobium d-orbitals dominate the electronic structure. The most stable isomer configurations are linear and cyclic structures, with the cyclic being the ground state for all but NbC<sub>6</sub>. To fully explain all experimental observations we are required to use the combined spectra of both ring and linear structures. This means that both structures must be present in the cluster beam, even in cases where the higher energy isomer is up to 0.5 eV higher than the ground state. This surprising result is confirmed by both DFT and Configuration Interaction.

1University of Southern Mississippi, Grant No. DE00945.

2This work has been funded by the Alexander von Humboldt Foundation.


4We gratefully acknowledge support from AFOSR grant #FA9550-05-1-0186 and #FA9550-07-1-0151.
2:34PM X37.00003 Photoelectron Velocity Map Imaging and Density-Functional Investigation of Bismuth and Lead Anions Solvated in Ammonia. KRISTEN CASALENUVO, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284, MOHAMED A. SOBH, Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802, J. ULISES REVELES, Department of Physics, Virginia Commonwealth University, UJJWAL GUPTA, Departments of Chemistry and Physics, The Pennsylvania State University, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, A.W. CASTLEMAN, JR., Departments of Chemistry and Physics, The Pennsylvania State University, SHIV KHANNA RESEARCH GROUP COLLABORATION, THE CASTLEMAN GROUP COLLABORATION — We present the results of photoelectron velocity map imaging experiments for the photodetachment of small negatively charged Bi, and Pb, \( n = 1-2 \) clusters solvated in ammonia using a Nd:YLF 527 nm laser. We report the vertical detachment energies of the observed multiple electronic bands and their respective anisotropy parameters derived from the photoelectron images. Density-functional theory calculations with generalized gradient approximation for the exchange-correlation potential were performed on these clusters to determine their molecular and electronic structures. Calculated ammonia binding energies and electronic charge transfers are used to rationalize the observed mass spectra distributions.

3:06PM X37.00004 Dielectric Phorephoresis and Dissociation of Micelles in AC-Electric Fields. VICTORIA FROUDE, YINGXI ELAINE ZHU, University of Notre Dame — Dielectrophoresis (DEP) of natural and synthetic colloids has been explored as a new route to rapidly manipulate and assemble colloidal particles in suspensions. Most work has been done with micron to submicron sized particles, yet AC-polarization and dielectric phorephoresis may provide facile methods to manipulate smaller particles. In this work we explore DEP and the dielectric phorephoresis of 10-100 nm polystyrene latex micelles. We find that the phorephoretic response of the micelles is modified by an AC field. This response can be tuned by the field strength and is sensitive to the micelle concentration, from which the DEP crossover frequency switching between the positive and negative DEP response is determined. Surprisingly, we also observe the AC-field induced dissociation of the micelle structure and the resultant release of fluorescent encapsulates at a characteristic low AC-field frequency of 1-10 kHz; the dissociation frequency can be tuned by encapsulated molecules with a strong dependence of their surface conductivity, which could have a potential application for controlled drug release by AC-electric fields.

3:18PM X37.00005 Raman Correlation Spectroscopy. MAKI NISHIDA, EDWARD VAN KEUREN, Georgetown University — We have developed a simple method for measurement of diffusion coefficients of specific components in complex mixtures of nanoparticles in a suspension. As a variation of Dynamic Light Scattering (DLS), this method analyzes temporal fluctuations of Raman scattered light from particles caused by Brownian motion. Due to the coherent nature of Raman scattering, the time autocorrelation functions of Raman emission lines will yield similar information as that obtained by DLS. Because each Raman emission line arises from a specific type of a molecular bond, only the diffusion coefficient of the particles containing that specific chemical species is measured. We demonstrate that this method can isolate diffusion coefficients from individual components in multicomponent nanoparticle dispersions.

3:30PM X37.00006 Nanosphere Templating Through Controlled Evaporation: A High Throughput Method For Building SERS Substrates. KRISTEN ALEXANDER, UNC Department of Chemistry, RENE LOPEZ, UNC Department of Physics, JOSEPH DESIMONE, UNC Department of Chemistry — When a pair of noble metal nanoparticles are brought close together, the plasmonic properties of the pair (known as a “dimer”) give rise to intense electric field enhancements in the interstitial gap. These fields present a simple yet exquisitely sensitive system for performing single molecule surface-enhanced Raman spectroscopy (SM-SERS). Problems associated with current fabrication methods of SERS-active substrates include reproducibility issues, high cost of production and low throughput. In this study, we present a novel method for the high throughput fabrication of high quality SERS substrates. Using a polymer templating technique followed by the placement of thiolated nanoparticles through meniscus force deposition, we are able to fabricate large arrays of identical, uniformly spaced dimers in a quick, reproducible manner. Subsequent theoretical and experimental studies have confirmed the strong dependence of the SERS enhancement on both substrate geometry (e.g. dimer size, shape and gap size) and the polarization of the excitation source.

3:42PM X37.00007 Resolving Single Molecule Dynamics with a Point-Functionalized Single-Walled Carbon Nanotube. DANNY W. WAN, ISSA S. MOODY, BRETT R. GOLDSMITH, JOHN G. CORONEUS, GREGORY A. WEISS, PHILIP G. COLLINS, Departments of Physics and Astronomy, Chemistry, Molecular Biology and Biochemistry, University of California, Irvine, CA 92697-4576 — We have achieved an unprecedented level of molecule-specific measurement of single molecule dynamics using a point-functionalized SWCNT electronic circuit [1]. Time-dependent components of the SWCNT conductance reveal real-time interactions between a covalently attached protein and the immediate electrodynamic environment. We will demonstrate electronic transduction of protein-substrate interactions with single molecule resolution. On-line analysis based on normalization of the power spectrum helps to enhance the resulting signals, even to the extent of providing the user with real time feedback regarding the experiment status. [1] B. Goldsmith et al, Science 315 77 (2007)

3:54PM X37.00008 Auger Rate Quenching in Nanocrystals. GEORGE E. CRAGG, Naval Research Laboratory, Washington, DC 20375, XIAOXI WANG, HUNG H. HU, Department of Chemistry, University of Rochester, Rochester, NY 14627, SARA MACCAGNANO-SCAGLIONE, ANDREW CHRISTIANSON, Oak Ridge National Laboratory, — We measured the far infrared vibrational properties of bulk and nanoscale MoS2 and MnO nanoparticles using the Photoelectron Velocity Map Imaging (P-VMI) technique. We find that the Auger rate suppression of the Auger rate has been suggested as the underlying mechanism for the non-blinking PL observed in soft-confinement, single CdZnSe/ZnSe NCs. To probe the interplay between the confinement geometry and the PL, we employ a coupled, two-band NC model which is analyzed with numerical routines based on the propagation matrix formalism. The results obtained will verify whether smooth confining potentials mitigate the Auger process, thereby eliminating blinking by allowing NCs to photoluminesce even in their charged state.
Ultrafast electronic energy redistribution in hollow gold nanoparticles. KENNETH KNAPPENBERGER, Florida State University, ADAM SCHWARTZBERG, LBNL — Nanostructured materials offer great potential for novel ways to generate, utilize, store and transport energy. These unique opportunities arise because nanoclusters often portray strikingly different chemical and physical properties than their bulk counterparts, and, perhaps more intriguingly, these vary widely with cluster size and shape. Here we report on the redistribution of electronic energy to thermal phonons in a series of hollow gold nanoparticles using femtosecond transient absorption. Qualitatively, the relaxation processes are similar to those of solid nanoparticles, however distinct differences are observed, likely owing to the unique properties of the hollow structures. In particular, a larger excitation power density is required to observe coherent vibrational oscillations in hollow gold nanoparticles than is needed for solid particles following electronic excitation. This effect is systematically studied over a range of hollow and solid particles, including multiple diameters and wall thicknesses. Models will be presented to account for the different relaxation mechanism observed for hollow and solid gold nanoparticles.

Optical spectra with spin-orbit effects on gold nanostructures. ALDO ROMERO, CINVESTAV, México, ALBERTO CASTRO, Institufur Theoretisch Physik, Freie Universitat Berlin, MIGUEL MARQUES, Université Lyon, France, MICAEL OLIVEIRA, University of Coimbra, Portugal, ANGEL RUBIO, ETSF, Universidad del País Vasco, Spain — The quest for more efficient optoelectronic devices requires a thorough understanding of the intrinsic properties of the metallic nanostructures such as the optical spectra. Many optoelectronic devices are based upon gold nanoparticles but even though, there is a large set of experimental studies, little is known theoretically. Between the concerns, it is important to identify where the spin-orbit effect has its optical spectra on the nanostructured materials. We report here the analysis of the effect of the spin-orbit interaction on the shape of the photoabsorption cross section of small gold clusters (Au$^+_n$, $n \leq 8$ and $n = 20$) and small nanowires ($n \leq 7$). As it is shown, the spin-orbit coupling has a strong effect on the absorption spectra mainly for nanowires and much less effect on static properties such as the dipole static polarizability. This has strong implications on transport calculations where no spin-orbit effects are considered.

First-principles studies of surface-enhanced Raman scattering: Benzene thiol on Au. ALEXEY ZAYAK, Department of Electrical Engineering and Computer Science, UC-Berkeley, CA, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA — First-principles calculations based on density functional theory are used to investigate how chemisorption of organic molecules on metal surfaces affects their Raman spectra. Experiments have long reported Raman intensity enhancements of orders of magnitude for molecules on rough metal surfaces or near nanofabricated metallic tips. The goal of this work is to explore "chemical" effects that may contribute to this enhancement, specifically hybridization and charge transfer between the molecule and its metallic substrate. We consider benzene thiol chemisorbed on extended Au(111) surfaces and finite Au and Ag clusters. Using a finite-difference scheme, we compute the absorption site, molecular orientation, and coverage dependence of Raman-active phonon modes and their intensities. We also examine how the electronic structure of the molecule is modified in each case, and discuss implications for the strength of Raman processes.

Photoluminescence anti-blinking of single CdZnSe/ZnSe nanocrystals. XI-AOYONG WANG, Department of Chemistry, University of Rochester, XIAOFAN REN, KEITH KAHEN, Eastman Kodak Company, MEGAN HAHN, Department of Chemistry, University of Rochester, MANJU RAJESWARAN, Eastman Kodak Company, SARA MACCAGNANO-ZACHER, JOHN SILCOX, School of Applied and Engineering Physics, Cornell University, GEORGE CRAGG, ALEXANDER EFROS, Naval Research Laboratory, TODD KRAUSS, Department of Chemistry, University of Rochester, UNIVERSITY OF ROCHESTER TEAM, EASTMAN KODAK COMPANY COLLABORATION, CORNELL UNIVERSITY COLLABORATION, NAVAL RESEARCH LABORATORY COLLABORATION — We have synthesized soft-confinement nanocrystals (NCS) of CdZnSe/ZnSe that on the single particle level exhibit complete elimination of photoluminescence (PL) blinking. These continuously emitting NCS have a very short PL decay lifetime of 5 ns. Moreover, single CdZnSe/ZnSe PL spectra are highly unusual with three distinct peaks. These unique and remarkable optical properties are collectively explained by the radiative recombination of a trion due to suppressed Auger processes in a NC. Upon deformation of the soft-confinement potential, the PL intensity of a single CdZnSe/ZnSe NC switches between two bright states, but still never turns off. Possible mechanisms for this PL anti-blinking behavior will be discussed.

Single-Electron Spectroscopy of Quantum Dots using Vertically Self-aligned Electrode Structure. RAMKUMAR SUBRAMANIAN, PRADEEP BHADRACHALAM, VISHVA RAY, SEONG JIN KOH, The University of Texas at Arlington — We demonstrate single-electron tunneling spectroscopy of individual quantum dots using new vertical electrode structure, where the source and drain electrodes are vertically self-aligned and separated by a thin dielectric spacer. A quantum dot placed on the periphery between the source and the drain electrodes forms a double barrier tunnel junction, allowing for single-electron spectroscopy measurements. CMOS compatible fabrication allows many quantum dot units to be fabricated in parallel processing. This technique not only provides an accurate electronic structure of a single quantum dot, but such measurement can be made for many of individual quantum dot units fabricated in a single batch process. Thus, this simple procedure provides a powerful tool to study quantum dot properties, and allows for the measurement of both the single and collective properties of quantum dots.

Thursday, March 19, 2009 2:30PM - 4:30PM
Session X38 DCP: Focus Session: Ion Channel Physics and Chemical Physics II
We have measured the global radiation sensitivity of model protein crystals as a function of temperature in the range 300 K to 100 K. Our data show three regimes, each characterized by a different activation energy for radiation damage being diffusion limited. Below 160 K, the activation energy is very small, and the cluster structure and individual channels are imaged simultaneously in a total internal reflection microscope. While most Kv2.1 channels in the cell are labeled with green fluorescent proteins (GFP), only a few individual channels are tagged with red quantum dots. This approach allows us to track single molecules and probe their interaction with the cluster perimeter. Different models for the molecular mechanism that localizes Kv2.1 clusters on the cell surface and the implications of our data will be discussed.

From 225 to 160 K, the activation energy is consistent with radiation damage being diffusion limited. Below 160 K, the activation energy is very small, and the cluster structure and individual channels are imaged simultaneously in a total internal reflection microscope. While most Kv2.1 channels in the cell are labeled with green fluorescent proteins (GFP), only a few individual channels are tagged with red quantum dots. This approach allows us to track single molecules and probe their interaction with the cluster perimeter. Different models for the molecular mechanism that localizes Kv2.1 clusters on the cell surface and the implications of our data will be discussed.

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Antifreeze proteins (AFP) and glycoproteins (AFGP) help fish, plants, insects and bacteria survive sub-freezing environments. It is well known that these proteins function via some surface interaction, but the exact mechanism has eluded scientists. Aside from mutagenesis experiments directed towards examining the functional importance of specific residues, conclusions about the mechanism have been drawn from indirect studies or more precisely from studies that describe the proteins effects on the ice interface. Our work is aimed at directly studying the protein kinetics at the ice/solution interface. Fluorescent microscopy is used to determine interaction planes, surface concentrations as well as adsorption characteristics and the segregation constants, while fourier transform infra-red attenuated total reectance (FTIR-ATR) is used to determine the protein structure vs. temperature in the liquid and solid states as well as the ice interface characteristics. All data show that AFGP do not function by the characteristic Gibbs-Thomson mechanism. While the surface coverage is similar for the AFPIII, segregation (amount in ice/amount in solution) is non-zero.

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3:30PM X39.00004 Ice-binding protein investigation using microfluidic devices

3:30PM X39.00005 Biominalization of a Self-Assembled Extracellular Matrix for Bone Engineering

4:06PM X39.00007 Superoxide dismutase activity of Cu-bound prion protein

4:18PM X39.00008 Mechanisms of function by AF(G)Ps in ice crystal growth prevention, modification and recrystallization

4:54PM X39.00009 Atomic Investigation of Cu-Induced Misfolding in the Onset of Parkinson's Disease
5:06PM X39.00010 ESR Spectroscopy Provides Direct Evidence of Cu$^{2+}$ Coordination by Three Histidine Residues in Aβ$_{1-10}$1. BYONG-KYU SHIN, SUNIL SAXENA, University of Pittsburgh — We provide direct evidence that all three histidine residues in amyloid-β$_{1-10}$ (Aβ$_{1-10}$) coordinate to Cu$^{2+}$. In our approach, we generate three Aβ$_{1-10}$ analogues, in each of which a selected histidine residue is isotopically enriched with $^{15}$N. Pulsed electron spin resonance (ESR) experiments such as electron spin echo envelope modulation (ESEEM) and hyperfine sublevel correlation (HYSCORE) clearly show that each of the three histidine imidazole rings at position 6, 13, and 14 in Aβ$_{1-10}$ binds to Cu$^{2+}$ as each of the three Cu$^{2+}$-$^{15}$N-labeled Aβ$_{1-10}$ complexes displays ESEEM and HYSCORE spectra which are distinctively different from those of the Cu$^{2+}$-nonlabeled Aβ$_{1-10}$ complex. The method employed here does not require either chemical side-chain modification or amino acid residue replacement, each of which is traditionally used to determine whether an amino acid residue in a protein binds to a metal ion. We also find that the histidine coordination in Aβ$_{1-10}$ is independent of the Cu$^{2+}$-to-peptide ratio, which is in contrast to the case of Aβ$_{1-40}$. The ESR results suggest tight binding between the histidine residues and the Cu$^{2+}$ ion, which is likely the reason of the high binding affinity of Aβ peptide to Cu$^{2+}$.

This work was supported by an NSF CAREER grant (MCB 0346898).

5:18PM X39.00011 Force Spectroscopy of Iron in Nitrosylated Hemes. J.T. SAGE, A. BARABANSCHIKOV, W. ZENG, Northeastern University, N.J. SILVERNAIL, W.R. SCHEIDT, Notre Dame University — Nitric oxide (NO) regulates important physiological processes by interacting with the Fe atom in heme proteins. We investigate the effect of NO binding on the local structure and dynamics of $^{57}$Fe by determining its vibrational density of states (VDOS), both experimentally, using nuclear resonance vibrational spectroscopy (NRVS) and computationally, using density functional theory (DFT). All Fe-ligand modes contribute to the VDOS, which provides uniquely quantitative information on the frequency, amplitude, and direction of the Fe motion. The VDOS also yields an experimental value for the stiffness, an effective force constant that probes nearest-neighbor interactions by measuring the force required to displace the Fe with the surrounding atoms fixed. Although vibrational mixing between Fe-NO stretching and FeNO bending character complicates structural interpretations of FeNO vibrations observed near 450 and 560 cm$^{-1}$, we find that the former mode contributes more strongly to the stiffness, indicating its sensitivity to the strength of the Fe-N bond. Comparison with DFT predictions identifies a feature observed near 130 cm$^{-1}$ in the VDOS of nitrosylated myoglobin as a vibration of the covalent link to the protein. We find that NO binding alters the interaction of the heme Fe with its local environment, and may facilitate NO recognition by heme proteins.

Thursday, March 19, 2009 2:30PM - 5:06PM — Session X40 DBP: Proteins in Membranes 412

2:30PM X40.00001 Copper coordination in the Glycine receptor by electron spin resonance. SHARON RUTHSTEIN, KATHERINE STONE, University of Pittsburgh, MICHAEL CASCIO, University of Pittsburgh School of Medicine, SUNIL SAXENA, University of Pittsburgh, SUNIL SAXENA’S GROUP TEAM, MICHAEL CASCIO’S GROUP TEAM — We describe the use of Electron Spin Resonance (ESR) to identify the coordination environment of copper in the extracellular domain of the protein, as well as the number of copper atoms that bind to Glycine receptor (GlyR). The GlyR channel mediates inhibitory neurotransmission in the central nervous system. It belongs to the superfamily of nicotinoid receptors. These receptors are formed by pentameric arrangement of subunits, each sharing a common topology having a large extracellular domain (ECD) and a transmembrane (TM) domain comprised of four membrane-spanning segments (TM1-TM4). For GlyR, four subunits (1-4) and one subunit have been identified to date, although the homomeric expression of just the α1 subunit of GlyR is sufficient to reconstitute native-like activity. The results are expected to shed light on the role of metals ion in modulating ion permeation in such receptor. In addition, an identification of copper binding sites will allow the measurement of large range distance constraints in the receptor by pulsed ESR. Such structural information on the GlyR in various allosteric states is essential in order to shed light on the gating mechanism of this protein membrane.

2:42PM X40.00002 Probing interaction of antimicrobial peptide duramycin with lipid monolayers. IZABELA I. RZEZNICKA, Riken, Advanced Science Institute, Wako-shi, Japan, MARIA SOVAGO, MISCHA BONN, Amolf, Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands, TOSHIHIDE KOBAYASHI, TARO YAMADA, Riken, Advanced Science Institute, Wako-shi, Japan, MAKIKAWAI, Riken, Advanced Science Institute, Wako-shi, Japan. Department of Advanced Materials Science, The University of Tokyo, Japan — Antimicrobial peptides are group of peptides which disrupt the microbial cell membrane through hydrophobic insertion into the outer lipid layer. Duramycin is a small tetracyclic peptide antibiotic, which has recently been shown to bind specifically to phosphatidylethanolamine (PE) lipids. We report the interaction of duramycin with phospholipid monolayers at air-water interface, studied using vibrational sum-frequency generation spectroscopy (VSFG) and fluorescence microscopy (FM). For monolayers containing PE lipids, VSFG reveals binding of duramycin to the monolayer through the appearance of a vibrational peak at 3045 cm$^{-1}$, corresponding to the C-H stretching vibration of phenylalanine amino acid. In addition, the amide I vibrational region shows that peptide has a β sheet conformation. Similar experiments performed on phosphatidylcholine (PC) monolayers show the interaction is specific with PE.

2:54PM X40.00003 Alamethicin Structure in Lipid Bilayers1. STEPHANIE TRISTRAM-NAGLE, JIAN-JUN PAN, Biol. Phys. Group, Physics Dept., Carnegie Mellon University, Pittsburgh, PA, JOHN NAGLE, Dept. Biol. Sci. and Physics Dept., Carnegie Mellon University, Pittsburgh, PA — This investigation uses x-ray diffuse scattering and MD simulations to study alamethicin (Alm) in fully hydrated bilayers of DOPC and diC22:1PC. Comparison of the experimental and simulated form factors supports the standard conclusion that Alm helices are inserted transmembrane along the bilayer normal at high humidity and high concentrations. Little change in membrane thickness with inserted Alm helices occurs for DOPC up to 1/10 Alm/DOPC. By contrast, the x-ray data strongly indicate that the diC22:1PC membrane, which is thicker than DOPC by 7 Å, thins with added Alm. Fitting the data to models of the electron density gives a decrease in thickness of 4 Å at 1/10 Alm/diC22:1PC. Although Alm’s helical length is close to the hydrophobic thickness of DOPC (27 Å), it is mismatched with the thicker diC22:1PC. Alm decreases the bending modulus (K$_{B}$) by a factor of ~2 in DOPC and a factor ~4 in diC22:1PC membranes at P/L ~1/10. Determination of the B modulus reveals a large increase in Hamaker parameter when Alm is added to diC22:1PC, but not to DOPC.

1This research was supported by NIH Grant No. GM 44976 and NIH/NIGMS under NSF award DMR-0225180 to CHESS.
behavior induced by these different peptides we will discuss the importance of amino acid composition and placement on membrane rearrangement.

The relationship between membrane composition and peptide induced changes in membrane curvature and topology is examined. By comparing the membrane phase transitions, we observe that the protein preferentially adsorbs on smaller vesicles, of diameter similar to the size of the bacterial spore ($\sim 1 \mu m$). Using fluorescent GFP-tagged SpoV, we quantify the amount of adsorbed protein by confocal microscopy. Our results, when interpreted using existing protein adsorption models, suggest the existence of a cooperative adsorption mechanism for high enough membrane curvature, which involves the formation of small clusters of proteins. Membrane curvature could be a general cue for protein localization in bacteria.

We thank a UMass Biomedical Innovation Initiative Grant and the NSF IGERT Program in Nanotechnology Innovation at the University of Massachusetts Amherst for funding.

We have developed several models to enhance our understanding of the effect of proteins in cell membranes, on phase separation, budding, and coarsening. In this work we investigate the effect of membrane hydration and hydrophobic mismatch on the Alm channel superstructure in an oriented multilayer sample by x-ray scattering. Wide angle x-ray (WAXS) scattering near 14 nm$^{-1}$ indicates that the lipid chain region is not perturbed much by the incorporation of up to 10 mole percent Alm. Low angle x-ray scattering (LAXS) indicates that when the sample is very dry, which promotes interactions between neighboring bilayers, a body centered tetragonal crystal packing of Alm channels is formed. As the hydration level increases closer to biological conditions, the separation between bilayers increases, the interbilayer interactions weaken, and the crystalline order disappears while considerable diffuse scattering remains. The effect of hydrophobic mismatch is examined for two mono-unsaturated lipids, diC18:1PC and diC22:1PC, that differ in bilayer thickness by 0.7nm. There is also in-plane scattering at a medium q of 7nm$^{-1}$ that our analysis suggests may not be from the Alm channel structure.

We thank a UMass Biomedical Innovation Initiative Grant and the NSF IGERT Program in Nanotechnology Innovation at the University of Massachusetts Amherst for funding.

Effects of Proteins and Lipids on Each Other in a Simulated Non-equilibrium Biomembrane Model. ANDREW P. PARADIS, University of Maine Department of Physics & Astronomy, SUSAN R. MCKAY, University of Maine Department of Physics & Astronomy, SAMUEL T. HESS, University of Maine Department of Physics & Astronomy, Institute for Molecular Biophysics — Lateral organization in biomembranes plays a major role in membrane topology, and is thus implicated in many basic functions of biomembranes such as endocytosis and signal transduction. In this study, non-equilibrium Monte Carlo simulations are used to investigate two related scenarios: 1. the effect of a rigid distribution of proteins on the lateral organization of lipids in a biomembrane, and 2. the degree to which lipid interactions influence the lateral organization of membrane-associated proteins that are free to translate laterally. Our model includes generic saturated and unsaturated lipids, proteins, and cholesterol, and is driven out of equilibrium through simulated endo- and exo-cytosis events. By varying the temperature, the protein mole fraction, and the interaction strengths, we examine the conditions under which various types of lateral organization occur. Simulation results are analyzed with pair-correlation functions and the Ripley K-test. We compare results from simulations of the two scenarios above and from simulations of biomembranes lacking protein.

Interactions of Defensins with Model Cell Membranes. LORI K. SANDERS, Dept. of Materials Science and Engineering, UIUC, NATHAN W. SCHMIDT, Dept. of Physics, UIUC, LIHUA YANG, ABHIJIT MISHRA, Dept. of Materials Science and Engineering, UIUC, MICHAEL E. SELSTED, Dept. of Pathology and Laboratory Medicine, UCI, GERARD C. L. WONG, Dept. of Materials Science and Engineering, UIUC — Antimicrobial peptides (AMPs) comprise a key component of innate immunity for a wide range of multicellular organisms. For many AMPs, activity comes from their ability to selectively disrupt and lyse bacterial cell membranes. There are a number of proposed models for this action, but the detailed molecular mechanism of selective membrane permeation remains unclear. Theta defensins are circularized peptides with a high degree of selectivity. We investigate the interaction of model bacterial and eukaryotic cell membranes with theta defensins RTD-1, BTD-7, and compare them to propeptin PG-1, a prototypical AMP, using synchrotron small angle x-ray scattering (SAXS). The relationship between membrane composition and peptide induced changes in membrane curvature and topology is examined. By comparing the membrane phase behavior induced by these different peptides we will discuss the importance of amino acid composition and placement on membrane rearrangement.
4:18PM X40.00010 Membrane fluidity in the presence of membrane-binding peptides, BEATRIZ BURROLA GABILONDO, WOLFGANG LOSERT, University of Maryland, PAUL RANDAZZO, National Cancer Institute — Arf proteins are GTPases that participate in vesicle trafficking inside cells. They are able to interact with membranes through their N-terminus when they are bound to GTP, and they detach from the membrane when GTP is hydrolyzed. The N-terminus of Arf1 (amino acids 2-17) folds into an amphiphilic helix that can insert into lipid bilayers. Arf1 is also myristoylated; it has myristic acid, a 14-carbon fatty acid 'tail', attached to it. We set out to test the hypothesis that the binding of the myristoylated N-terminus of Arf1 to lipid membranes changes the mechanical properties of the membrane, in ways that myristic acid alone or amphotropic peptides alone do not. We use three reporter molecules embedded in vesicles, whose fluorescence emission spectrum depends on the properties of the environment in which they are found, to measure three distinct aspects of membrane fluidity: Bispynene is sensitive to lateral motion along the membrane, Prodan's emission gives a measure of the packing of the head groups, and DPH polarization reflects the packing of the hydrophobic tails. We will present effects found for four molecules (myristic acid, myristoylated and non-myristoylated N-terminus of Arf1, and the ALPS domain of KES) in a concentration-dependent manner, and discuss the importance of these results in the vesicle-trafficking picture.

4:30PM X40.00011 New insights into the bacterial cell wall peptidoglycan architecture, JOHN DUTCHER, AHMED TOUHAMI, University of Guelph, MANFRED JERICHO, Dalhousie University — The molecular architecture of the bacterial cell wall peptidoglycan (saccu) is among the most challenging, yet still unsoled, structural problems in biochemistry. Two models have been proposed: the planar model, in which the glycan strands lie in the plane of the cell surface, and the scaffold model, in which the glycan stands lie perpendicular to the cell surface. We have used atomic force microscopy (AFM) to investigate the molecular structure of this unique biopolymer in the rod-shaped bacterium Bacillus subtilis at high resolution. AFM images recorded in air on single saccu revealed a porous regular network with 25-50 nm-wide peptidoglycan fibers and a 5-25 nm pore size. Interestingly, the new bacterial pole showed a regular structure with the same fiber sizes but with the fibers running in a direction that is almost perpendicular to that observed away from the pole. This finding combined with our previous data on live hydrated bacteria (1) provides new insights into the three-dimensional architecture of the peptidoglycan of Gram-positive bacteria. 1- A. Touhami, M. H. Jericho, and T. J. Beveridge, J. Bacteriol., 2004 186: 3266-3295.

4:42PM X40.00012 An Analytic Study of Molecular Motion in Cell Membranes, ZIYA KALAY, Consortium of the Americas for Interdisciplinary Science and Dept. of Engineering and Mechanics, Univ. of New Mexico, Albuquerque, NM USA, LUCA GIUGGIOLI, Dept. of Engineering and Mechanics, Univ. of New Mexico, Albuquerque, NM USA, AMAL PARRIS, Missouri Univ. of Science and Technology, Rolla, MO, USA, VASUDEV KENKREV, Consortium of the Americas for Interdisciplinary Science and Dept. of Physics, Univ. of New Mexico, Albuquerque, NM USA — We present a theoretical calculation to describe the confined motion of transmembrane molecules in cell membranes. Understanding the motion of membrane-associated molecules, e.g. various types of receptors, has great modern relevance in cell biology. Our study is divided into two parts. In the first, we consider motion in an ordered system and in the second, we investigate the effects of disorder by employing an effective medium approximation. Both are based on Master equations for the probability of the molecules moving as random walkers, and leads to explicit usable solutions including expressions for the molecular mean square displacement and effective diffusion constants. As a result, the calculations make possible, in principle, the extraction of confinement parameters such as mean compartment sizes and mean intercompartmental transition rates from experimentally reported published observations.

4:54PM X40.00013 Detergent interaction with tethered bilayer lipid membranes for protein reconstitution, MATTEO BROCCIO, HAW ZAN GOH, MATHIAS LOESCHE, Carnegie Mellon University — Tethered bilayer lipid membranes (TBLMs) are self-assembled bimolecular layers in which the membrane is separated from a solid substrate by a nm-thick hydrated submembrane space. These model systems are being used in binding studies of peripheral proteins and exotoxins. Here we aim at their application for the reconstitution of water-insoluble integral membrane proteins. As an alternative to fusion of preformed protosomites we study the direct reconstitution of such proteins for applications in biophysics. In particular we show that TBLMs (DOPC – DOPG) were temporarily incubated with a detergent to screen for conditions that keep the detergent-saturated membrane stable and ready to incorporate detergent-solubilized proteins. We assess the electrical characteristics, i.e. specific resistance and capacitance, by means of electrochemical impedance spectroscopy (EIS) under timed incubation with deacylalyzed and deoxycholate detergents in a regime around their critical micelle concentration, 1.8 mM and 0.17 mM respectively and demonstrate the restoration of the TBLM upon detergent removal. Thereby a range of concentration and incubation times was identified, that represents optimal conditions for the subsequent membrane protein reconstitution.

Thursday, March 19, 2009 2:30PM - 4:42PM — Session X41 DMP DCMP: Strongly Correlated Electrons 413

2:30PM X41.00001 Breakdown of the BCS Ground State at a Quantum Phase Transition, RAFAEL JARAMILLO, The University of Chicago, YEJUN FENG, Advanced Photon Source, THOMAS ROSENBAUM, The University of Chicago, JONATHAN LANG, ZAHIR ISLAM, GEORGE SIMON ( IListed in alphabetical order), PETER LITTLEWOOD, Cambridge University — We use hydrostatic pressure to suppress the magnetism in elemental chromium, a simple cubic metal that demonstrates a subtle form of itinerant antiferromagnetism, formally equivalent to the BCS state in superconductors. By directly measuring the associated charge order with x-ray diffraction in a diamond anvil cell at low temperatures, we reveal a continuous magnetism in elemental chromium, a simple cubic metal that demonstrates a subtle form of itinerant antiferromagnetism, formally equivalent to the BCS state in superconductors. We use three reporter molecules embedded in vesicles, whose fluorescence emission spectrum depends on the properties of the environment in which they are found, to measure three distinct aspects of membrane fluidity: Bispynene is sensitive to lateral motion along the membrane, Prodan’s emission gives a measure of the packing of the head groups, and DPH polarization reflects the packing of the hydrophobic tails. We will present effects found for four molecules (myristic acid, myristoylated and non-myristoylated N-terminus of Arf1, and the ALPS domain of KES) in a concentration-dependent manner, and discuss the importance of these results in the vesicle-trafficking picture.

2:42PM X41.00002 Ultrafast photo-induced spin and charge dynamics in correlated electron system, SUMIO ISHIHARA, YU KANAMORI, Department of Physics, Tohoku University, HIROAKI MATSUEDA, Sendai National College of Technology — Photo-induced phenomena in correlated electron system are one of the attractive themes in recent solid state physics. One of the well known examples is magnetism with the perovskite crystal structure. The charge ordered insulating state associated with the antiferromagnetic (AFM) long-range order competes with the ferromagnetic metallic phase. After introduction of the pump photon into the charge-ordered insulating phase, dramatic changes in the optical reflectivity and in the optical Kerr rotation are observed. These results imply that the charge and magnetic structures are changed cooperatively by the photo-irradiation. We present a theoretical study of photo-induced dynamics in a correlated electron system where electronic charge couples with spin and lattice. The generalized double exchange model is analyzed by utilizing the two complementary methods, the exact diagonalization and inhomogeneous Hartree-Fock methods. Time evolutions of the optical absorption spectra, spin correlation, and charge correlation are calculated. There are two time scales in the photo-induced dynamics; the charge and AFM spin orders are collapsed within a short time scale corresponding to 10-100 fs, and the long-range FM spin correlation appears in a long time scale corresponding to a few ps.
3:06PM X41.00004 Probing orbitons in YTiO3 with Resonant Inelastic X-ray Scattering, LUCAS AMENT, Lorentz Institute, Leiden, GINIYAT KHALILULLIN, Max Planck Institute, Stuttgart, JEROEN VAN DEN BRINK, Lorentz Institute, Leiden — In YTiO₃, a strongly correlated electron system with degenerate orbitals, orbitons are predicted to exist [1]. The hallmark of collective excitations is dispersion. To observe the orbiton dispersion, the rapidly developing technique of Resonant Inelastic X-ray Scattering (RIXS) is especially well suited. We analyze recent experimental RIXS data on YTiO₃ in the Ultrashort Core hole Lifetime framework [2]. The Ti ions in this material have a 3d⁹ configuration, and the electron occupies one of the three degenerate t₂g orbitals. Many of this compound’s ground state properties are explained by assuming that the orbitals on these Ti ions talk to each other through a superexchange mechanism [1]. RIXS could couple to the orbital excitations (orbitons) in these kinds of materials in two ways: via modification of the superexchange interactions [3] and via a shakeup process. We compare our theoretical RIXS spectra to experimental ones, giving strong evidence for the existence of orbitons. // [1] G. Khalilullin and S. Okamoto, Phys. Rev. B 68, 205109 (2003) // [2] J. van den Brink and M. van Veenendaal, Europhys. Lett. 73, 121 (2006); L. J. P. Ament, F. Forte and J. van den Brink, Phys. Rev. B 75, 115118 (2007) // [3] compare F. Forte, L. J. P. Ament and J. van den Brink, PRL (2008)

3:18PM X41.00005 Polaronic hole-trapping in doped insulating oxide, CESARE FRANCHINI, GEORG KRESSE, RAIMUND PODLOUCKY, University of Vienna — In transition-metal oxides, local electronic correlation effects dominate the physics, and lattice degrees of freedom are often only treated as external perturbations. However, in systems dominated by s and p electrons, electronic correlation is expected to be less important, and in agreement with this conjecture, we show that lattice degrees of freedom are crucial to account for the hole doping driven insulator-to-metal/superconducting transition (IMT) in Ba₁₋ₓKₓBiO₃. Specifically, by using hybrid-DFT we show that Bi⁵⁺ sites trap two holes from the valence band accompanied by a large local lattice distortion, commonly referred to as bipolaronic state. We show that in pure Bi₃BiO₅ a single peak in the imaginary part of the dielectric function is visible which corresponds to the charge-ordered excitation between Bi⁵⁺ and Bi⁵⁺ sub-bands. Upon hole-doping a second peak emerges at x = 0.125 connected with the bipolaronic excitation. At x = 0.25 the bipolaronic peak increases in intensity and is shifted towards lower energy, thus indicating the incipient IMT observed at x ≈ 0.3. Our results describe all relevant experimental results.

3:30PM X41.00006 Systematic enhancement in magnetic susceptibilities and a study of Fermi Liquid behavior of Re₂Ta₁₀ where Re=Y and La, and T =Fe, Ru, and Os¹, KEESEONG PARK, YURI JANSEN, MOOSUNG KIM, Brookhaven National Laboratory, CARLOS MARQUES, Stony Brook University, MEIGAN ARONSON, Brookhaven National Laboratory — DC and AC magnetic susceptibilities, specific heat and resistivity are measured for YbFe₂Al₁₀-structure compounds, Re₂Ta₁₀ where Re=Y, and La, and T =Fe, Ru, and Os. The YT₂Al₁₀ show mean-field superconducting behavior in magnetic properties from Os to Ru and to Fe, and Fermi-liquid behaviour below around 100 K. With the linear term of the specific heat (γ₀) and the temperature independent susceptibility (χ₀) at low temperature, the Stoner enhancement parameter, Z, is utilized to find how close the compounds are to the ferromagnetic ordering, where Z = 1-(β₆/2γ₀²)穀γ₀/χ₀穀. Specifically, YFe₂Al₁₀ shows a larger Z (0.98) than that (0.83) of Pd, a well known example of nearly ferromagnetic materials. The implied proximity to the quantum criticality is tested by a power law analysis, where 1/(χ₀ − χ₀) =AT⁴ can describe well a wide range (2K to 100K) of AC magnetic susceptibility for YFe₂Al₁₀ with λ = 1.19, which is between the mean-field value (λ = 1) and that of the three-dimensional Ferromagnetic Heisenberg model (λ = 1.33).

¹Work at Brookhaven performed under the auspices of the Department of Energy Office of Basic Energy Science

3:42PM X41.00007 Soliton Wall Superlattice Charge-Density-Wave Phase in Quasi-One-Dimensional Conductor (Per)₂Pt(mnt)₂², SI WU, ANDREI LEBED, University of Arizona — We demonstrate that the Pauli’s spin splitting effects in a magnetic field improve nesting properties of a realistic quasi-one-dimensional electron spectrum. As a result, a high resistance Peierls charge-density-wave (CDW) phase is stabilized in high enough magnetic fields in (Per)₂Pt(mnt)₂ conductor. We show that, in low and very high magnetic field, the Pauli spin-splitting effects lead to a stabilization of a soliton wall superlattice (SWS) CDW phase, which is characterized by periodically arranged soliton and anti-soliton walls. We suggest experimental studies of the predicted first order phase transitions between the Peierls and SWS phases to discover a unique SWS phase. It is important that, in the absence of the magnetic field and in the limit of very high magnetic field, the suggested model is equivalent to the exactly soluble model of Brazovskii, Dzyaloshinskii, and Kirova.

²This work was supported by the NSF Grant DMR-0705986.

3:54PM X41.00008 Non Fermi Liquid behavior and disorder in BaVS₃, ANA AKRAP, Brookhaven National Laboratory, Upton, New York, NEVEN BARISIC, Universitaet Stuttgart, Germany, FLORENCE RULLIER-ALBENQUE, SPEC, Orme des Merisiers, CEA, GIF sur Yvette, France, HELMUTH BERGER, LASZLO FORRO, Institut de Physique de la matiere complexe, EPFL, Lausanne, Switzerland — In strongly correlated BaVS₃, the interplay between a wide one-dimensional d² band and the localized ν₁ electrons leads to a wealth of electronic phases. In this work we investigate the high pressure non-Fermi liquid (NFL) phase of BaVS₃ by means of transport measurements, focusing on the influence of disorder, introduced by fast electron irradiation and sulfur deficiency. Our results are interpreted within a novel scenario in which quasi-one-dimensional 2kF-CDW fluctuations are responsible for the NFL behavior [3].

³N. Barisić et al., arXiv:0712.3393v1

4:06PM X41.00009 The role of charge degrees of freedom in Mott insulators: coupling of dielectric and magnetic properties in Cr-trimer complexes, ROSS MCDONALD, OSCAR AYALA VALENZUELA, MARCELO JAIME, NHMFL-Los Alamos, JOHN MYDOSH, University of Koln — Materials that are insulating owing to strong electron correlations are pervasive in condensed matter physics—the parent phase of high-Tc cuprates, colossal magnetoresistive manganites and quantum magnets. All are characterized by a large onsite Coulomb repulsion relative to the dominant electron hopping. As such, at half-band filling the charge is localized. The independent properties of these materials are therefore controlled solely in terms of their spin degrees of freedom, with little attention given to any further role of the charge. Certain classes of Mott insulator are predicted to break this paradigm, providing a direct correlation between the magnetic spin texture and the dielectric properties of a material. We observe such a correlation in Cr-trimer systems, which combined with recent theoretical developments, indicates a purely electronic mechanism for multiferroic behavior. Magnetic field strengths of the order of the exchange interaction strongly perturb the spin texture, which is evident as steps and plateau in the magnetization. The corresponding shifts in dielectric properties reveal the role of the charge degrees of freedom. Electron Spin Resonance (ESR) results and the prospect of novel dipole-active ESR giving rise to the possibility of negative refractive indices will also be discussed.

4:18PM X41.00010 The Jahn-Teller effect in doped LiCuO₂, CHRIS MARIANETTI, Columbia University — LiCuO₂ displays one of the largest known Jahn-Teller distortions, where Cu⁺⁺ is in a low spin configuration. Previous density functional theory (DFT) calculations verified the fact that the high spin, non-Jahn-Teller distorted LiCuO₂ is a metastable phase. In this work, we use DFT calculations to demonstrate that doping this system with ions that are not Jahn-Teller active allows one to tune the energy difference between the high-spin, non-Jahn-Teller phase and the low-spin, Jahn-Teller phase. This occurs due to the elastic penalty of the non-Jahn-Teller ion in the Jahn-Teller phase. The effect of different non-Jahn-Teller dopants is presented, and the electronic nature of the two respective phases is detailed.
10:24AM Y1.00005 Thermally activated phase slips in superconducting nanowires. VINCENT DUBOST, University of Paris, CRISTIAN VAJU, Institut des Materiaux Jean Rouxel, TRISTAN CREU, University of Paris, BENNOU CORRAZI, Institut des Materiaux Jean Rouxel, FRANCOIS DEBONTRIDDER, University of Paris, ETIENNE JANOD, Institut des Materiaux Jean Rouxel, DIMITRI RODITCH, University of Paris, LAURENT CARIO, Institut des Materiaux Jean Rouxel, INSP DISPOSITIFS QUANTIQUES CONTROLES TEAM, IMN-PMN-MATERIAUX A PROPRIETES ELECTRONIQUE NON-CONVENTIONNELLES TEAM. We have recently discovered a bulk Electric Pulse Induced Insulator-Metal Transition and possible superconductivity in the cluster Mott Insulator GaTaeSe8. The transport measurements, conducted on single crystals, are consistent with a two-channel model, which suggests that the electric pulse generates electronic inhomogeneities in the bulk of the samples. Our Scanning Tunneling Microscopy (STM) experiments indeed confirmed the observed drop in the resistance which was interpreted as a superconducting transition driven by a Mott transition. The signature of the Mott transition is the appearance of quantum fluctuations which were detected by analyzing the tunneling current fluctuations. The tunneling current contains information on the electronic properties of the sample. The Mott transition is observed as a suppression of the tunneling current fluctuations which indicates that the sample becomes insulating. The suppression of the current fluctuations is observed for a wide range of temperatures and also for a wide range of voltages. The current fluctuations are associated with the interplay of the Mott transition and the superconducting transition. The interplay of the two transitions leads to a new universal behavior which is observed in the tunneling current fluctuations. The universal behavior is characterized by a new exponent which is different from the exponents observed in the classical Mott transition and the superconducting transition. The new exponent is related to the interplay of the two transitions. The new exponent is related to the nature of the Mott transition and the superconducting transition. The new exponent is related to the nature of the Mott transition and the superconducting transition. The new exponent is related to the nature of the Mott transition and the superconducting transition.

This work was supported by DOE grant DE-FG02-07ER46453.
8:36AM Y2.00002 Differential Dynamic Microscopy: a simple means to measure dynamics with a microscope, ROBERTO CERBINO, Universita degli Studi di Milano — Optical microscopy is an excellent tool to investigate the structure and dynamics of soft and biological materials. In this contribution we present a novel scheme to measure the dynamics of a system using an ordinary microscope [1]. This scheme is based on the spatial Fourier analysis of a time series of microscopy images, which enables us to study the relaxation of the intensity Fourier components at different spatial frequencies. This quantifies the dynamic activity of the system at different wave-vectors, giving access to information similar to the one obtained in dynamic light scattering experiments. Our technique termed Differential Dynamic Microscopy (DDM) is capable of monitoring the dynamics of both objects that are larger and smaller than the wavelength of light. The remarkable simplicity of DDM makes it suitable for the use in any laboratory that is equipped with an ordinary microscope.

Ref:

9:12AM Y2.00003 Holographic video microscopy, DAVID GRIER, New York Univ NYU — No abstract available.

9:48AM Y2.00004 New techniques for fluorescence background rejection in microscopy and endoscopy, CATHIE VENTALON, Laboratory of Neurophysiology and New Microscopies, CNRS UMR 8154, INSERM S603, University Paris Descartes - 45 rue des Saints Pères - 75006 Paris — Confocal microscopy is a popular technique in the bioimaging community, mainly because it provides optical sectioning. However, its standard implementation requires 3-dimensional scanning of focused illumination throughout the sample. Efficient non-scanning alternatives have been implemented, among which the simple and well-established incoherent structured illumination microscopy (SIM) [1]. We recently proposed a similar technique, called Dynamic Speckle Illumination (DSI) microscopy, wherein the incoherent grid illumination pattern is replaced with a coherent speckle illumination pattern from a laser, taking advantage of the fact that speckle contrast is highly maintained in a scattering media, making the technique well adapted to tissue imaging [2]. DSI microscopy relies on the illumination of a sample with a sequence of dynamic speckle patterns and an image processing algorithm based only on an a priori knowledge of speckle statistics. The choice of this post-processing algorithm is crucial to obtain a good sectioning strength: in particular, we developed a novel post-processing algorithm based one wavelet pre-filtering of the raw images and obtained near-confocal fluorescence sectioning in a mouse brain labeled with GFP, with a good image quality maintained throughout a depth of ~100 μm [3]. In the purpose of imaging fluorescent tissue at higher depth, we recently applied structured illumination to endoscopy. We used a similar set-up wherein the illumination pattern (a one-dimensional grid) is transported to the sample with an imaging fiber bundle with miniaturized objective and the fluorescence image is collected through the same bundle. Using a post-processing algorithm similar to the one previously described [3], we obtained high-quality images of a fluorescein-labeled rat colonic mucosa [4], establishing the potential of our endomicroscope for bioimaging applications.

Ref:

10:24AM Y2.00005 Photoactivated localization microscopy combined with single particle tracking, SULIANA MANLEY, NICHD — No abstract available.

Friday, March 20, 2009 8:00AM - 11:00AM – Session Y3 DCMP: Multi-valley Electron Systems in the Quantum Limit 301/302

8:00AM Y3.00001 Phase Transitions of Dirac Electrons in Bismuth1, LU LI2, Physics Department, Princeton University, Princeton, NJ 08544 — The Fermi Surface (FS) in elemental bismuth consists of 3 electron ellipsoids and one hole ellipsoid [1]. The accidental coincidence of the hole and electron caliper areas when the field \( H \) is aligned with the trigonal axis \( Z \) has long stymied analyses of the quantum oscillations. Because of current strong interest in how electrons with Dirac dispersion behave in intense fields, we have renewed attack on this problem [2] using high-resolution torque magnetometry in fields up to 31 T and at temperatures \( T \) down to 300 mK. When \( H \) is tilted with respect to \( Z \) by a slight angle \( \theta \), the torque \( \tau \) on the sample derived from the 3 electron ellipsoids dominates the torque from the hole FS, allowing the Landau Level crossings of the Dirac electron to be resolved. By measuring the curves of \( \tau \) vs. \( H \) at 19 values of \( \theta \) straddling the trigonal axes, we completely resolve the Landau Levels of the Dirac electrons. A new result is the detection of jumps in the transverse magnetization when \( H \) exceeds the quantum limit of the electron pockets. By tracing the jumps in the plane of \( H \) vs. \( \theta \), we uncover a region in which the Dirac electrons enter a new ground state. Within this cone-shaped region, Landau Level anomalies are severely suppressed. We interpret the state as one in which the 3-fold valley degeneracy of the Dirac gas is lifted to form a many-body state. The unusual nature of the magnetization within this region will be described.

Ref:

1Research partially supported by NSF-MRSEC Grant (DMR 0213706). High-field experiments were performed at the National High Field Magnet Lab., Tallahassee, which is supported by NSF, DOE and the State of Florida.

2Current address: Physics Department, MIT, Cambridge, MA 02139
8:36AM Y3.00002 Hall Plateaus at magic angles in ultraquantum Bismuth. FAUQUE BENOIT, Laboratoire Photon et Matière — The behaviour of a three-dimensional electron gas in the presence of a magnetic field strong enough to put all carriers in the first Landau level (i.e. beyond the quantum limit) is a longstanding question of theoretical condensed matter physics [1]. This issue has been recently explored by two high-field experiments on elemental semi-metal Bismuth. In a first study of transport coefficients (which are dominated by hole-like carriers), the Nernst coefficient presented three unexpected maxima that are concomitant with quasi-plateaux in the Hall coefficient [2]. In a second series of experiments, torque magnetometry (which mainly probes the three Dirac valley electron pockets) detected a field-induced phase transition [3]. The full understanding of the electron and hole behaviours above the quantum limit of pure Bi is therefore still under debate. In this talk, we will present our measurement of the Hall resistivity and torque magnetometry with magnetic field up to 31 T and rotating in the trigonal-bisectrix plane [4]. The Hall response is dominated by the hole pockets according to its sign as well as the period and the angular dependence of its quantum oscillations. In the vicinity of the quantum limit, it presents additional anomalies which are the fingerprints of the electron pockets. We found that for particular orientations of the magnetic field (namely “magic angles”), the Hall response becomes field-independent within the experimental resolution around 20T. This drastic dependence of the plateaux on the field orientation provides strong constraints for theoretical scenarios.

References:

9:12AM Y3.00003 Bismuth and graphite in the ultraquantum limit: signatures of fractional quantum Hall effect. YAKOV KOPELEVICH, Instituto de Física “Gleb Wataghin”, Universidade Estadual de Campinas, UNICAMP, Campinas, Brasil — Bismuth and graphite are semimetals that possess both conventional massive and Dirac-like quasiparticle spectra. High quality graphite is a multi-layer system with nearly decoupled two-dimensional (2D) graphene planes, in which the integer quantum Hall effect has already been found [1]. On the other hand, the fractional quantum Hall effect (FQHE) has been observed for 3D bismuth in the ultraquantum limit (UCL), i.e. above the field that pulls all carriers into the lowest Landau level [2]. Recent measurements performed on quasi-2D graphite in magnetic field up to B = 57 T revealed well defined plateaus in the Hall resistance for B > 10 T, suggesting also the FQHE occurrence in graphite in the UCL [3]. A striking similarity of the obtained results with the FQHE measured for 2D electron system in a GaAs/AlGaAs quantum well [4] is found. Our present results indicate the interplay between FQHE and charge density wave states in graphite. We discuss the FQHE occurrence in bismuth and graphite within the framework of available theoretical models.

References:

9:48AM Y3.00004 AlAs 2D Electrons at High Magnetic Field: The Role of Spin and Valley Degree of Freedom. MANSOUR SHAYEGAN — Two-dimensional (2D) electrons in AlAs quantum wells occupy multiple conduction-band minima (or valleys) at the X point of the Brillouin zone. These valleys have large effective mass (m*e) and g-factor compared to the standard GaAs electrons, and are also highly anisotropic. The system is rather unique in that, with proper choice of well width and by applying in situ symmetry-breaking strain in the plane, one can control the occupation of different valleys, thus rendering a system with tuneable m*e, g-factor, Fermi contour anisotropy, and with single, double, or triple valley degeneracy. By adding a magnetic field, we obtain a system which allows us to explore very rich physics ensuing from the valley and spin degrees of freedom in a strongly interacting system. In this presentation, I will highlight some of our latest results on 2D electrons confined to wide AlAs quantum wells where the electrons reside in two in-plane valleys whose occupation can be controlled via the application of strain. I will present the results of our m*e measurements, via analyzing the temperature dependence of the Shubnikov-de Haas oscillations. The measured m*e shows a strong dependence on the occupation of valley and spin subbands, reflecting the electron-electron interaction in this system. Most remarkably, m*e is suppressed with respect the band value when the 2D electrons are fully spin- and valley-polarized. I will also discuss the relation of m*e suppression to the 2D metal-insulator transition problem. Our studies also include measurements of the valley susceptibility (dependence of valley population on applied strain) and the valley polarization of the fractional quantum Hall effect composite fermions. While part of our observations can be explained well by a simple Landau level fan diagram for composite fermions with a valley degree of freedom, there are some surprises.


10:24AM Y3.00005 High Mobility Sixfold Valley Degenerate Electrons on Silicon [111] Surfaces, ROBERT N. MCFARLAND, Laboratoy for Physical Sciences, University of Maryland, College Park — The 111 surface of silicon is predicted to retain the sixfold valley degeneracy of the ideal bulk crystal. We have developed a method for fabricating field effect transistors using vacuum as a dielectric in order to study electron transport on the bare hydrogen-terminated surface, free from the complications created by intrinsic disorder at Si-Si interfaces. The resulting devices display very high mobilities (up to 110,000 cm²/Vs at 70K, more than twice as large as the best silicon MOSFETs), enabling us to probe valley-dependent transport dynamics to a much greater degree than previously possible. Measurements made on a recent device over a density range of n,c = 0.7 – 7 x 10¹⁵/cm² reveal considerable information about the nature of this degeneracy and its role in 2D transport. In particular, we find (at n,c = 6.7) that 1) low field Shubnikov-de Haas oscillations reveal a clearly sixfold degenerate system and allow us to establish an upper bound on the valley splitting of 0.2K 2) longitudinal resistivity at B=0 displays a strong temperature dependence, consistent with predictions that large valley degeneracy should enhance screening[1] and 3) the Hall coefficient near B=0 is modified by the presence of multiple valleys, and we can use this correction to measure the intervalley Coulomb drag and its temperature dependence. [1] E. H. Hwang and S. Das Sarma. PRB 75, 073301 (2007)

1This work was performed in collaboration with Tomasz M. Kott, Luyan Sun, and Bruce E. Kane of the Laboratory for Physical Sciences, University of Maryland at College Park and Kevin Eng of Sandia National Laboratories.
8:00AM Y4.00001 Neutron and X-Ray Scattering Studies of the Exchange Bias Problem. SUNIL K. SINHA, Department of Physics, University of California, San Diego — Exchange Bias, i.e. the shift of the hysteresis loop of a ferromagnet in juxtaposition to an antiferromagnet, is a phenomenon that has been known for fifty years, and has already been put to wide commercial use in devices such as magnetic read-heads and other devices. Nevertheless a detailed understanding of the effect has proved to be fairly controversial, notwithstanding much research on this problem over the years, and the development of several alternative theoretical models. This is partly due to the necessity of understanding the details of the interactions and the magnetic structure across and in the vicinity of the interface between the ferromagnet and the antiferromagnet. The details of how interface roughness and other defects affect exchange bias and the details of how magnetic domains are established on both sides of the interface are still not well understood. Non-destructive probing of such buried interfaces is conveniently accomplished with neutron scattering or synchrotron X-ray techniques such as X-Ray Magnetic Circular Dichroism, Photoemission imaging or Resonant Magnetic X-ray Scattering, and these types of experiments have been increasingly employed over the last decade. We shall attempt to discuss what has been learned from such experiments and what crucial issues remain unresolved, with particular emphasis on recent studies of the Co/Fe and Permalloy/CoO exchange bias bilayer systems.

8:36AM Y4.00002 Measuring interfacial magnetic configurations with Polarized Neutron Reflectometry. THOMAS HAUET, Hitachi GST — Polarized neutron reflectivity (PNR) is ideally suited for imaging both vertical structural and magnetic variations in the complex magnetic multilayers [1]. During the talk will be described particularly how this technique allows obtaining the magnetic depth-profile of exchange-coupled bilayer. For instance, Gd60Fe40/Tb12Fe88 is a model system to study exchange-bias phenomena origin in anti-ferromagnetically coupled AF/FM system, like FeF2/Fe. In these systems, unusual properties are observed such as a transition from positive to negative exchange bias field HE as the cooling field Hc is swept from small to large positive value [2]. Combining complementary techniques that are macroscopic magnetization measurements and PNR, we have demonstrated that the above properties, e.g. the cooling field dependence of HE, come from an interfacial domain wall (IDW) frozen in the TbFe as the sample is cooled down under a field [3, 4]. Moreover, PNR measurements have recently revealed that the frozen IDW is metastable and that the exchange bias training effect in TbFe/GdFe results from the thermally assisted relaxation of the IDW, with field cycling [4, 5]. Overall, PNR studies concerning the TbFe/GdFe have brought strong insights into the exchange bias mechanisms in exchange coupled hard/soft systems with in-plane anisotropy. However we have demonstrated as well that this powerful technique can be applied to systems with perpendicular magnetic anisotropy (PMA). Although, in that case, the perpendicular moments are parallel to the scattering vector and do not give rise to scattering via the neutron selection rules, we have used a unconventional geometry to obtain a depth-dependent magnetic profile of a PMA exchange-coupled system. Specifically, we have characterized antiferromagnetically-coupled, TbFeCo/[Co/Pd] multilayers [6].

References

9:12AM Y4.00003 Inelastic neutron scattering studies of exchange biased core-shell nanoparticles. MIKHAIL FEYGENSON, Brookhaven National Laboratory — Inelastic neutron scattering (INS) measurements of nanoparticle systems are very few, and we report here the first investigation of exchange biased core-shell nanoparticles. We present a study of spin dynamics in core-shell Co/CoO nanoparticles, which display an exchange bias field of 0.6T. We have used INS measurements to determine how the magnetic dynamics are affected, both by the onset of antiferromagnetic (AF) order at 250K and the subsequent onset of the exchange bias effect at 200K. At the highest temperatures, the scattering consists of two quasielastic peaks. The narrower peak is ascribed to superparamagnetic reorientations of the Co core. The broader peak originates with moments in the CoO shell. Surprisingly, their dynamics speed up with decreasing temperature, suggesting that the CoO shell absorbs some of the magnetic energy of the core as exchange blocking is approached. Below 200K, the scattering is dominated by an inelastic peak at ~3meV. The integrated spin wave intensity grows when the temperature is reduced below 200K, reaches a maximum near 150K, and nearly vanishes at the low temperatures. We attribute this peak to AF spin waves in the CoO shell, and their lack of dispersion and overall energy scale are consistent with predictions for low energy spin waves in bulk CoO [3,4]. It is remarkable that bulk-like spin wave behavior is observed in the CoO shell, which is only 4 nm thick.

References

9:48AM Y4.00004 Exchange bias in core/shell magnetic nanoparticles: experimental results and numerical simulations. XAVIER BATLLE, Dep. Fisica Fonamental and Institut de Nanociencia i Nanotecnologia IN2UB, Universitat de Barcelona, Catalonia, Spain — In this talk, we will review some of the main experimental observations related to the occurrence of exchange bias in magnetic systems, focusing the attention on the phenomenon appearing in nanoparticles with core/shell structure as compared to thin film bilayers [1]. The main open questions posed by the experimental observations will be discussed and contrasted to existing theories and models for exchange bias [1]. We will also present some recent numerical simulations [2-4] based on a simple model of a core/shell nanoparticle, showing evidence that the magnetic order of interfacial spins accounts for most of the experimental observations. Finally, we will discuss the occurrence of exchange bias on laser-ablated granular thin films composed of Co nanoparticles embedded in amorphous zirconia matrix [5]. The deposition method allows controlling the degree of oxidation of the Co particles by tuning the oxygen pressure at the vacuum chamber. The nature of the nanoparticles embedded in the magnetic multilayer may be monitored from metallic, ferromagnetic (FM) Co to antiferromagnetic (AFM) CoOx, with a FM/AFM intermediate regime for which the percentage of the AFM phase can be increased at the expense of the FM phase, leading to the occurrence of exchange bias in particles of about 2 nm in size. This is a model system to study some of the features of exchange bias in nanoparticles, such as particle size dependence, induced exchange anisotropy on the FM leading to high irreversible hysteresis loops, and blocking of the AFM clusters due to proximity to the FM phase.

References
1. For a recent review see, for example, “Exchange bias phenomenology and models of core/shell nanoparticles”; Iglesias, O.; Labarta, A.; and Batlle, X. Journal of Nanoscience and Nanotechnology 8, 2761 (2008).

Work at Brookhaven National Laboratory was performed under the auspices of US Department of Energy Office of Basic Energy Sciences.

Work in collaboration with: A. Labarta, O. Iglesias, M. Garcia del Muro and M. Kovylina. The funding from the Spanish MEC (MAT2006-03999, NAN2004-08805-C04-02, and CONSOLIDER CSD2006-12), and from the Catalan DURSI (2005SGR00969) is acknowledged.
10:24AM Y4.00005 Small-Angle Neutron Scattering Studies of Magnetic Correlation Lengths in Nanoparticle Assemblies, SARA MAJETICH, Carnegie Mellon University — Small-angle neutron scattering (SANS) measurements of ordered arrays of surfactant-coated magnetic nanoparticle reveal characteristic length scales associated with interparticle and intraparticle magnetic ordering. The high degree of uniformity in the monodisperse nanoparticle size and spacing leads to a pronounced diffraction peak and allows for a straightforward determination of these length scales [1]. There are notable differences in these length scales depending on the particle moment, which depends on the material (Fe, Co, Fe3O4) and diameter, and also on whether the metal particle core is surrounded by an oxide shell. For 8.5 nm particles containing an Fe core and thick Fe3O4 shell, evidence of a spin flop phase is seen in the magnetite shell when a field is applied, but not when the shell thickness is ~0.5 nm [2]. 8.0 nm particles with an e-Co core and 0.75 nm CoO shell show no exchange bias effects while similar particles with a 2 nm thick shell show significant training effects below 90 K. Polarized SANS studies of 7 nm Fe3O4 nanoparticle assemblies show the ability to resolve the magnetization components in 3D.


Friday, March 20, 2009 8:00AM - 11:00AM
Session Y5 DBP: Self-Organization in Biological Cells and Tissues II 401/402

8:00AM Y5.00001 Cells anticipate periodic events, TOSHIYUKI NAKAGAKI, RIES, Hokkaido University — We show that an amoeboid organism can anticipate the timing of periodic events. The plasmodium of the true slime mold Physarum polycephalum moves rapidly under favourable conditions, but stops moving when transferred to less-favourable conditions. Plasmodia exposed to unfavourable conditions, presented in three consecutive pulses at constant intervals, reduced their locomotive speed in response to each episode. When subsequently subjected to favourable conditions, the plasmodia spontaneously reduced their speed at the time point when the next unfavourable episode would have occurred. This implied anticipation of impending environmental change. After this behaviour had been evoked several times, the locomotion of the plasmodia returned to normal; however, the anticipatory response could subsequently be induced by a single unfavourable pulse, implying recall of the memorized periodicity. We explored the mechanisms underlying these behaviours from a dynamical systems perspective. Our results hint at the cellular origins of primitive intelligence and imply that simple dynamics might be sufficient to explain its emergence.

8:36AM Y5.00002 The Physics of Cardiac Fibrillation: Strings that kill1, EBERHARD BODENSCHATZ, MPI for Dynamics and Self-Organization — Fibrillation is a state of spatio-temporal chaos in a 3d-biological excitable medium, namely the heart muscle. The building blocks are wave-emitting three-dimensional topological singularities in the electric excitation field of the tissue. These string like singularities send out rotating wave fields with very fast frequencies (up to 10 times normal heart rate) and thus dominate over the pacemaker. The incoherent electrical excitation of the spatio-temporal chaotic dynamics leads to an unsynchronized contraction of the cardiac muscle and to the loss of the pumping action, and if untreated to death. Due to the topological nature of the spatio-temporal chaotic state it is very difficult to control. Current defibrillation technologies use strong electric field pulses (1 kV, 30 A, 12 ms) to reset the whole muscle. Here we report that natural muscle heterogeneities act as wave emitting sites when a weak electric field pulse is applied across the tissue. We report theoretical predictions on the physics and support the findings by results from experiment. This work was conducted in collaboration with Stefan Luther (MPIDS), Falvio Fenton (Cornell), Amgad Squires (Cornell), Robert Gilmour (Cornell), Valentin Krinsky (MPIDS), Alain Pumir (Nice).

1Supported by MPG and NIH.

9:12AM Y5.00003 Spatiotemporal patterns of voltage and calcium signaling in heart cells and tissue, ALAIN KARMA, Department of Physics and CIRCS, Northeastern University, Boston, USA — This talk will describe recent progress made in understanding oscillatory patterns of voltage and calcium signals that precede the onset of electromechanical wave turbulence in the main chambers of the heart. Results will illustrate how both physiologically detailed and abstract models have proven useful to cope with the bewildering molecular complexity of cardiac biology and to bridge phenomena on cellular and tissue scales. A main conclusion is that those oscillatory patterns can be self-organized, resulting from symmetry-breaking linear instabilities, or/and a manifestation of underlying tissue heterogeneities. Thus studying the evolution of those patterns provides a valuable indirect probe of complex physiological processes that render the heart susceptible to the sudden onset of lethal heart rhythm disorders.

9:48AM Y5.00004 Synchronization of Eukaryotic Flagella and the Evolution of Multicellularity1, RAYMOND GOLDSTEIN, University of Cambridge — Flagella, among the most highly conserved structures in eukaryotes, are responsible for such tasks as fluid transport, motility and photoaxisis, establishment of embryonic left-right asymmetry, and intercellular communication, and are thought to have played a key role in the development of multicellularity. These tasks are usually performed by the coordinated action of groups of flagella (from pairs to thousands), which display various types of spatio-temporal organization. The origin and quantitative characterization of flagellar synchronization has remained an important open problem, involving interplay between intracellular biochemistry and interflagellar mechanical/hydrodynamic coupling. The Volvocine green algae serve as useful model organisms for the study of these phenomena, as they form a lineage spanning from unicellular Chlamydomonas to germ-soma differentiated Volvox, having as many as 50,000 biflagellated surface somatic cells. In this talk I will describe extensive studies [1], using micromanipulation and high-speed imaging, of the flagellar synchronization of two key species - Chlamydomonas reinhardtii and Volvox carteri - over tens of thousands of cycles. With Chlamydomonas we find that the flagellar dynamics moves back and forth between a stochastic synchronized state consistent with a simple model of hydrodynamically coupled noisy oscillators, and a deterministic one driven by a large interflagellar frequency difference. These results reconcile previously contradictory studies, based on short observations, showing only one or the other of these two states, and, more importantly, show that the flagellar beat frequencies themselves are regulated by the cell. Moreover, high-resolution three-dimensional tracking of swimming cells provides strong evidence that these dynamical states are related to reorientation events in the trajectories, yielding a eukaryotic equivalent of the “run and tumble” motion of peritrichously flagellated bacteria. The degree of synchronization is found to depend upon the presence of external fluid flow, an important aspect of the dynamics in the context of evolutionary transitions to multicellularity. Comparison is made with dynamics of somatic cells of Volvox, which we have found can display metachronal waves, not previously reported in this organism. Implications of these findings for phototactic steering are also discussed.


1Supported by EPSRC, BBSRC, HFSP, Marie-Curie, and the Schlumberger Chair Fund
10:24AM Y5.00005 Novel orbital physics with fermions in optical lattices. 

KCONJUN WU, Department of Physics, University of California, San Diego — Orbitals, a degree of freedom characterized by orbital degeneracy and spatial anisotropy and independent of change and spin, play important roles in magnetism and superconductivity in transition metal oxides. In this talk, we will show that the rapid progress of cold atom physics has opened up an opportunity to study novel features of orbital physics, which do not appear usual solid state systems. In particular, the \( p_{\pm 3} \)-orbital system of the honeycomb lattice exhibits amazingly rich and fundamentally different behavior from that in the \( p_{\pm 3} \)-orbital system of graphene. Its flat band structure dramatically interacts with other bands and provides a natural way to study non-perturbative strong correlation phenomena such as Wigner crystallization, and ferromagnetism which is an important field in condensed matter physics but has not attracted much attention in the cold atom community. Furthermore, in the Mott-insulating states, the orbital degree of freedom enables superexchange interactions as spin does. We will show how spatial anisotropy generates frustration in such systems, which leads to a promising way to the exciting orbital liquid states. At last, we will present that a topological insulating phase occurs in the presence of the lattice rotation, as an orbital analog of the quantum anomalous Hall effect of electron systems.

References:

This work was supported by Sloan Research Foundation, NSF-DMR-0804775, and ARO-W911NF0810291.

Friday, March 20, 2009 8:00AM - 11:00AM –
Session Y6 DCMP DAMOP: Novel Orbital Quantum Phases in Cold Atom Optical Lattices

8:00AM Y6.00001 Dynamics of ultracold atoms in higher lattice orbitals. 

TORBEN MUELLER, Institute for Quantum Electronics, ETH Zurich, Switzerland — Ultracold quantum gases in far detuned optical lattices have enabled many intriguing experiments studying a new regime of strongly correlated quantum systems. So far, such experiments have mostly concentrated on atoms in the vibrational ground state of the lattice band structure. Here, we report on the realization of a multi-orbital system with ultracold atoms in the excited bands of a 3D optical lattice by selectively controlling the band population along a given lattice direction. The lifetime of the atoms in the excited band is found to be considerably longer (10-100 times) than the characteristic time scale for intersite tunneling, thus opening the path for orbital selective many-body physics with ultracold atoms in optical lattices. Upon exciting the atoms from the initial lowest band Mott-insulating state to higher lying bands, we observe the dynamical emergence of long-range coherence in 1D (and also 2D) at nonzero quasimomentum, providing a possible route for Bose-Einstein condensation to nonzero momentum.

8:36AM Y6.00002 Control of Bosons in a 2D optical lattice with checkerboard staggered field. 

TREY PORTO, NIST — I will describe experiments to control the vibrational and spin degrees of freedom of ultra-cold Rb atoms in a novel 2D optical lattice. This unit cell of the lattice can be dynamically transformed between a single-site and two-site configuration, allowing us to manipulate the vibrational degree of freedom of atoms in the unit cell, and merge separated atoms into the same site. In addition, the vector light shift of the optical lattice acts as a Zeeman field for the atoms on every other site of the lattice, providing a checkerboard staggered field. We use this field to control the spins on the two sub-lattices separately. I will also discuss the possibility of using this field to prepare low entropy anti-ferromagnetic states.

This work was partially supported by IARPA and ONR.


W. VINCENT LIU, University of Pittsburgh — Bose-Einstein condensation (BEC) is often associated with zero momentum to which a macroscopic fraction of bosons condense. Here we propose a new class of meta-stable quantum states where bosons condense at non-zero momenta, defying the paradigm. This becomes possible when bosonic atoms are confined in the \( p \)-orbital Bloch bands of an optical lattice rather than the usual \( s \)-orbital. A recent experiment at Mainz confirmed the discovery of such an exotic BEC with alkali-metal atoms in a 3D cubic lattice with anisotropic optical potentials. Non-zero momentum suggests crystalline order. Our theoretical studies further found that such non-zero momentum BECs are also naturally orbital ordered superfluids due to the fascinating, less studied center-of-mass \( p \)-wave symmetry (e.g., a vortex-like \( p_x + ip_y \) condensate). Varying with the geometry from standard optical lattices to double-well lattices, the interesting orderings include staggered orbital currents, stripes of angular momenta, and modulated super-current density wave. Different than a phase of coexisting orders such as supersolidity, this new class of states is characterized by a single order parameter. Work done in collaboration with J. Moore, S. Das Sarma, V. M. Stojanovic, C. Wu, and E. Zhao.

References:

This work was supported by ARO (W911NF-07-1-0464) and DARPA (OAR ARO W911NF-07-1-0993).


CONJUN WU, Department of Physics, University of California, San Diego — Orbitals, a degree of freedom characterized by orbital degeneracy and spatial anisotropy and independent of change and spin, play important roles in magnetism and superconductivity in transition metal oxides. In this talk, we will show that the rapid progress of cold atom physics has opened up an opportunity to study novel features of orbital physics, which do not appear usual solid state systems. In particular, the \( p_{\pm 3} \)-orbital system of the honeycomb lattice exhibits amazingly rich and fundamentally different behavior from that in the \( p_{\pm 3} \)-orbital system of graphene. Its flat band structure dramatically interacts with other bands and provides a natural way to study non-perturbative strong correlation phenomena such as Wigner crystallization, and ferromagnetism which is an important field in condensed matter physics but has not attracted much attention in the cold atom community. Furthermore, in the Mott-insulating states, the orbital degree of freedom enables superexchange interactions as spin does. We will show how spatial anisotropy generates frustration in such systems, which leads to a promising way to the exciting orbital liquid states. At last, we will present that a topological insulating phase occurs in the presence of the lattice rotation, as an orbital analog of the quantum anomalous Hall effect of electron systems.

References:

We thank the support from Sloan Research Foundation, NSF-DMR-0804775, and ARO-W911NF0810291.
10:24AM Y6.00005 Realization of Extended Hubbard Models with Tailored Orbitals in Optical Lattices\textsuperscript{1}, VITO SCAROLA, UC Berkeley — Optical lattices containing cold atoms represent nearly ideal manifestations of Hubbard models free from disorder, defects, impurities and lattice phonons. Experiments with bosonic alkali atoms confined to the lowest optical lattice band demonstrate strongly correlated phases including the superfluid and Mott insulator that arise from a real space contact interaction between atoms. Can other quantum condensed phases of matter be observed in these systems? We show that promoting bosons to higher bands effectively extends the range of the contact interaction. Quasi-localized orbitals in higher bands overlap with nearest neighbors. They can be modeled with extended Bose-Hubbard models that harbor density wave and supersolid phases. Bosons promoted to higher bands can decay but the purity of optical lattice systems limits possible decay mechanisms (e.g. phonons). We propose that long-lived metastable states of bosons promoted to higher bands of optical lattices may therefore provide a route to a novel class of extended Hubbard models.

\textsuperscript{1}Work done at the University of Maryland in collaboration with S. Das Sarma and supported by ARO-DARPA.

Friday, March 20, 2009 8:00AM - 11:00AM –
Session Y7 GSNP DCMP: The Statistical Properties of Forc...
10:24AM Y7.00005 Measuring the configurational temperature of granular media, MATTHIAS SCHRÖTER, Max Planck Institute for Dynamics and Self-Organization — Twenty years ago Edwards and Oakeshott suggested developing a statistical mechanics of static granular media based on the idea that the logarithm of the number of mechanically stable states of a specific sample constitutes the relevant entropy [1]. From this entropy then, a configurational temperature, named compactivity, could be derived. However, in the absence of an appropriate thermometer to measure compactivity, the question if it is indeed a relevant state variable remained untested. Only recently it was shown that the steady state volume fluctuations of a periodically driven sample can be used to measure the compactivity of a granular sample including its dependence on volume fraction and surface friction of the particles [2]. This opens up the possibility of studying questions like the existence of a zeroth law of granular thermodynamics or the relationship between compactivity and other forms of granular temperature.


Friday, March 20, 2009 8:00AM - 11:00AM – Session Y8 GIMS: Pushing the Limits of Mechanical Detection 414/415

8:00AM Y8.00001 Quantum Optical Control of Micromechanics, MARKUS ASPELMEYER, Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences, Vienna, Austria — Massive mechanical resonators are now approaching the quantum regime. This opens up not only a spectrum of new applications but also a previously inaccessible parameter range for macroscopic quantum experiments on optomechanical entanglement, which is at the heart of Schrödinger’s cat paradox.

8:36AM Y8.00002 Measurement of Dispersive Coupling Between a Nanoresonator and a Superconducting Qubit, MATTHEW LAHAYE, California Institute of Technology — Incorporating superconducting qubit technology into nano-electromechanical systems (NEMS) should enable the observation of quantum behavior in NEMS. Ultimately, it is expected that coupled qubit-NEMS systems could serve as a test bed for studying fundamental issues of quantum mechanics including the quantum limits of measurement and the quantum-classical divide. Proposals in the literature posit the qubits as verifiable toolboxes for preparing, manipulating and measuring quantum states of a nanomechanical resonator (or ‘nanoresonator’), and range from the nondestructive read-out of quantized-energy states (or ‘Fock states’) to the generation of Schrödinger-cat states. In an initial step toward implementing these advanced strategies, we have performed the first measurements of a nanoresonator coupled to a superconducting qubit, the Cooper-pair box (CPB). We find that the coupling produces a CPB-state-dependent shift in the frequency of the nanoresonator that is analogous to the single-atom phase shifts experienced by superconducting resonators in the dispersive limit of cavity quantum electrodynamics (CQED). In my talk, I will report on our latest measurements of the dispersive interaction between the CPB and nanoresonator, including how we utilize it to read-out quantum interference effects in the CPB. In the end, I will discuss how the interaction could soon be utilized for exploring the quantum limit of NEMS.

9:12AM Y8.00003 Nanoscale Magnetic Resonance Imaging Based on Ultrasensitive Force Detection1, H.J. MAMIN, IBM Research Division, Almaden Research Center — Magnetic Resonance Force Microscopy (MRFM) seeks to dramatically improve the sensitivity and resolution of magnetic resonance imaging (MRI), perhaps ultimately down to the molecular scale. It uses force detection to circumvent the sensitivity limits inherent in conventional inductively-detected MRI. By using an ultrasensitive, single crystal silicon cantilever cooled to 300 mK, we can detect forces smaller than 1 aN, allowing us to sense the magnetism from small ensembles of nuclear spins. We have used tobacco mosaic virus as a test object, detecting the hydrogen signal. Using three-dimensional scans and mathematical deconvolution algorithms, we have made 3D reconstructions of the viruses with resolution down to roughly 4 nm. This represents a 10^6 x improvement in minimum detectable volume compared to the best conventional MRI. Advancing the technique further will require reducing the force noise, increasing the achieved magnetic field gradients, and making use of the inherent chemical sensitivity of magnetic resonance.

1Work done in collaboration with Christian Degen, Martino Poggio, Charles Rettner, Tjerk Oosterkamp, Mark Sherwood and Dan Rugar

9:48AM Y8.00004 A Cantilever-based apparatus for detecting micron-scale deviations from Newtonian gravity1, AHARON KAPITULNIK, Stanford University — To test new theories of physics beyond the Standard Model, we have built a low temperature probe to measure forces as small as 10^{-18} N between masses separated by distances on the order of 20 microns. Our experiment is fundamentally a Cavendish-type experiment in the sense that its purpose is to directly measure the force between two masses [1]. A cryogenic helium gas bearing is used to rotate a disc containing a drive mass pattern of alternating density under a small test mass mounted on a micromachined cantilever. Any mass-dependent force between the two will produce a time-varying force on the test mass, and consequently a time-varying displacement of the cantilever. This displacement is read out with a laser interferometer, and the position of the drive mass is simultaneously recorded using an optical encoder. The displacement is then averaged over many cycles and converted to a force using measured properties of the cantilever. This AC “lock-in” type measurement enables significant noise rejection and allows us to operate on resonance to take advantage of the cantilever’s high quality factor. A novel feature of the apparatus is the utilization of feedback regulation of the response of the microcantilever using the radiation pressure of a laser. Our approach does not require a high-finesse cavity, and the feedback force is due solely to the momentum of the photons in the second laser.


1Work was done in collaboration with D. Weld, J. Xia, B. Cabrera and T.J. Bay. This work was supported by NSF grant number PHY-054170.

10:24AM Y8.00005 The quantum limit and beyond in gravitational wave detection, NERGIS MAVALVALA, Massachusetts Institute of Technology — The sensitivity of current and next generation interferometric gravitational wave detectors is limited by quantum mechanics. We will explore this quantum limit, one aspect of which arises from the radiation pressure that laser light exerts on the movable mirrors of the interferometer. I will describe experiments in which the light force dominates the mechanical forces to such an extent that the mirror oscillators are optically trapped and cooled. Laser cooling of macroscopic mechanical oscillators has applications in high precision force and position measurements, gravitational wave detection, and exploration of the classical-quantum boundary. I will discuss the status of a variety of experimental efforts worldwide are working to approach the quantum regime, with the goal of observing non-classical effects such as quantum back-action, squeezing and entanglement of the light and mirror states, and conclude with an outlook on prospects for observation of quantum effects in macroscopic human-scale objects.

Friday, March 20, 2009 8:00AM - 10:48AM – Session Y9 GSNP: Stochastic Processes in Biological Systems II 303
8:00AM Y9.00001 A Stochastic Single-Molecule Event Triggers Phenotype Switching of a Bacterial Cell, SUNNEY XIE, PAUL CHOI, Harvard University, LONG CAI, Caltech — By monitoring fluorescently labeled lactose permease with single-molecule sensitivity, we investigated the molecular mechanism of how an Escherichia coli cell with the lac operon switches from one phenotype to another. At intermediate inducer concentrations, a population of genetically identical cells exhibits two phenotypes: induced cells with highly fluorescent membranes and uninduced cells with a small number of membrane-bound permeases. We found that this basal-level expression results from partial dissociation of the tetrmeric lactose repressor from one of its operators on looped DNA. In contrast, infrequent events of complete dissociation of the repressor from DNA result in large bursts of permease expression that trigger induction of the lac operon. Hence, a stochastic single-molecule event determines a cell’s phenotype.

1Current address

8:12AM Y9.00002 The role of time scales in extrinsic noise propagation, SRIVIDYA IYER-BISWAS, Dept. of Physics, The Ohio State University, JUAN MANUEL PEDRAZA, Dept. of Systems Biology, Harvard Medical School, C. JAYAPRAKASH, Dept. of Physics, The Ohio State University — Cell-to-cell variability in the number of proteins has been studied extensively experimentally. There are many sources of this stochastic variability or noise that can be classified as intrinsic, due to the stochasticity of chemical reactions and extrinsic, due to environmental differences. The different stages in the production of proteins in response to a stimulus, the signaling cascade before transcription, transcription, and translation are characterized by different time scales. We analyze how these time scales determine the effect of the reactions at each stage on different sources of noise. For example, even if intrinsic noise dominates the fluctuations in mRNA number, for typical degradation rates, extrinsic noise can dominate corresponding protein number fluctuations. Such results are important in determining the importance of intrinsic noise at earlier stages of a genetic network on the products of subsequent stages. We examine cases in which the dynamics of the extrinsic noise can lead to differences from cases in which extrinsic noise arises from static (in time) cell-to-cell variations. We will interpret the experiments of Pedraza et al. in the light of these results. *J. M. Pedraza et al, Science 25 March 2005: Vol. 307. no. 5717, pp. 1965 - 1969.

8:24AM Y9.00003 Determination of the equilibrium free energy for pulled single molecules from nonequilibrium work measurements1, LIAO CHEN, University of Texas at San Antonio — The Jarzynski equality (JE) is widely accepted for extracting equilibrium free energy from non-equilibrium work measured in single-molecule pulling experiments, even though questions remain on its validity and applicability. In this talk, I will show that the JE is actually inapplicable outside the near-equilibrium regime. We present a new fluctuation-dissipation theorem (FDT) that is derived within the context of Brownian dynamics. The new FDT agrees with the JE in the near equilibrium regime but it is valid in far nonequilibrium regime where the JE does not stand. In silico experiments of unfolding polypeptides show that the new FDT is indeed accurate for far non-equilibrium processes.

1Supported in part by TACC and by NIH (GM084834)

8:36AM Y9.00004 Efficient stochastic sampling of first passage times for multi-scale simulations, NAVODIT MISRA, RUSSELL SCHWARTZ, Carnegie Mellon University — Monte Carlo methods have become increasingly popular for simulating stochastic dynamics in biological systems. However, the standard Stochastic Simulation Algorithm (SSA) can become highly inefficient for multi-timescale problems, where important events occur in parallel and at a much slower rate than other relatively unimportant events. We present two new algorithms based on the spectral analysis of Continuous Time Markov Model (CTMM) graphs to achieve fast rare event sampling in SSA models. These methods are well suited for simulating a broad class of ‘stiff’ reaction networks such as models of bond networks and nucleation-limited self-assembly in biological systems.

8:48AM Y9.00005 Dynamics of segregation of polymers in a confined geometry, YA LIU, BULBUL CHAKRABORTY, Brandeis University — Chromosomes are enormous DNA molecules living in the crowded, confined environment of a cell. They carry important genetic information and are stably propagated to new generations through replication. During the replication, two identical DNA molecules are generated and segregate rapidly into opposite pole of the cell. We have used numerical simulation to investigate the effects of confinement on the segregation of two identical self-avoiding chains. Simulation shows the existence of a transition from a mixing state to a demixing state with changes in the confining geometry. Using the blob picture, we construct a free energy function that depends on the distance between the two chains. We describe the dynamics of segregation as a stochastic process driven by this energy function. We will present comparisons of our theoretical results with numerical simulations.

9:00AM Y9.00006 Modeling DNA unhooking from a single post as a translocation process, NABIL LAACHI, JAESOOL CHO, KEVIN DORFMAN, University of Minnesota-Twin Cities — We will present theoretical results on the stochastic unhooking of a long DNA chain from an isolated, stationary micropillar obtained by mapping the unhooking process to the translocation of a long chain through a nanopore. We show how stochastic methods, developed for DNA translocation, can thus be utilized to study chain-post unhooking. In particular, implementing such methods leads to the full probability distribution of the unhooking time and the ensuing moments in a fast and efficient manner for a wide range of chain and field parameters. The results thus obtained compare favorably to more realistic (and computationally intense) Brownian Dynamics simulation data, indicating that the finite size of the insulating micropillar and the elasticity of the DNA make at most a small contribution to the dynamics. We will also address the relevant electric fields and time scales for this process, making a connection between the theoretical data obtained here and experimental separations.

9:12AM Y9.00007 Evolutionary advantage of a mixed strategy for the competence phenotype in bacteria, CHRISTOPHER WYLIE, HERBERT LEVINE, UC San Diego, DAVID KESSLER, Bar Ilan University, CENTER FOR THEORETICAL BIOLOGICAL PHYSICS TEAM — Under certain stressful conditions, bacterial species such as B. subtilis undergo a differentiation process in which a finite subpopulation transiently and stochastically enters the “competent” state. This state is defined by the ability to import and homologously incorporate extracellular DNA fragments into the genome. This ability is accompanied by a growth rate that tends to slow adaptive evolution. On the other hand, the increased genetic diversity generated by recombination tends to speed evolution. Using stochastic simulation and analytic methods, we show that this tradeoff implies that a “mixed strategy” optimizes the rate at which populations acquire beneficial mutations.

9:24AM Y9.00008 Physical limits on computation by assemblies of allosteric proteins1, JOHN ROBINSON, University of Alabama at Birmingham — Assemblies of allosteric proteins are the principle information processing devices in biology. Using the Ca2+-sensitive cardiac regulatory assembly as a paradigm for Brownian computation, we examine how system complexity and system resetting impose physical limits on computation. Nearest-neighbor-limited interactions among assembly components constrains the topology of the system’s macrostate free energy landscape and produces degenerate transition probabilities. As a result, signaling fidelity and deactivation kinetics can not be simultaneously optimized. This imposes an upper limit on the rate of information processing by assemblies of allosteric proteins that couple to a single ligand type.

1Supported by NIH, ESF
9:36AM Y9.00009 Calcium waves in the maturing oocyte
t. AMAN ULLAH, Ohio University, GHANIM ULLAH, The Pennsylvania State University, PETER JUNG, Ohio University, KHALED MACHACA, Weill Cornell Medical College, Qatar — Calcium waves in oocytes are sustained by release of Ca\textsuperscript{2+} from the endoplasmic reticulum (ER) through clustered release channels. As the oocytes mature, a) the calcium waves slow down by about a factor of two, b) the overall duration of Ca\textsuperscript{2+} elevation grows substantially, and c) the cell is more susceptible to wave initiation. At the same time, the kinetics of release of Ca\textsuperscript{2+} from a single cluster is changed only insignificantly. Based on a computational model that accurately reproduces elemental Ca\textsuperscript{2+} release kinetics from channel clusters, we propose that the changing spatial organization of signaling effectors is a common underlying cause for all the above described observations as the Ca\textsuperscript{2+} signaling machinery matures.
1This work was supported by NSF.

9:48AM Y9.00010 Calcium puffs: From microdomain to a channel. DIVYA SWAMINATHAN, PETER JUNG, Department of Physics and Astronomy, Ohio University — Calcium puffs describe the release of calcium (Ca\textsuperscript{2+}) ions from internal stores into the cytosol through clusters of up to tens of ion channels. It is believed that during the release process, when the channels open, steep Ca\textsuperscript{2+} concentration gradients are established around the cluster. These local large concentrations are consequential as they determine the opening and closing rates of the ion channel and therefore control receptor kinetics. We present a computational study, wherein we simulate the release and diffusion of Ca\textsuperscript{2+} ions and its interaction with buffers and indicator dyes around one channel cluster. Our goal is to relate local steep Ca\textsuperscript{2+} gradients with experimentally observable microdomain-averaged Ca\textsuperscript{2+} concentrations thereby putting the high concentration hypothesis to test.

10:00AM Y9.00011 Dynamical Phase Transitions In Periodically Driven Model Neurons R. ENGBRECHT\textsuperscript{1}, RENATO MIROLLO\textsuperscript{2}, Physics\textsuperscript{1} and Mathematics\textsuperscript{2} Departments, Boston College — Transitions between dynamical states in integrate-and-fire (IF) neuron models with periodic stimuli result from tangent or discontinuous bifurcations of a return map. We study their characteristic scaling laws and show that discontinuous bifurcations exhibit a new kind of phase transition intermediate between continuous and first order. We then consider a much more complicated Hodgkin-Huxley type of model and show that in the presence of periodic stimuli an attracting 2D invariant subspace develops in the 7D state space. A Poincare section on this subspace yields a 1D return map, remarkably similar to the IF case. This reduction to 1D map dynamics should extend to real neurons in a periodic current clamp setting.

10:12AM Y9.00012 Stochastic and Deterministic Flagellar Dynamics Provide a Mechanism for Eukaryotic Swimming Reorientation MARCO POLIN, IDAN TUVAL, KNUT DRESCHER, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — The biflagellated alga *Chlamydomonas reinhardtii* is a good model organism to study the origin of flagellar synchronization. Here we employ high-speed imaging to study the beating of the two flagella of *Chlamydomonas*, and show that a single cell can alternate between two distinct dynamical regimes: asynchronous and synchronous. The asynchronous state is characterized by a large interflagellar frequency difference. In the synchronous state, the flagella beat in phase for long periods, interrupted episodically by a large difference in frequency difference. The statistics of these events are consistent with a model of hydrodynamically coupled noisy oscillators. Previous observations have suggested that the two flagella have well separated intrinsic beat frequencies, and that they are synchronized by their mutual coupling. Our analysis shows instead that the synchronized state is consistent with coupling-induced synchronization of flagella with those intrinsic frequencies. This suggests that the beat frequencies themselves are under the control of the cell. Moreover, high-resolution three-dimensional tracking of swimming cells provides strong evidence that these dynamical states are related to non-phototactic reorientation events in the trajectories, yielding a eukaryotic equivalent of the "run and tumble" motion of peritrichously flagellated bacteria.

10:24AM Y9.00013 Active stochastic oscillations and amplification of mechanical stimuli in a hair cell model LIJUAN HAN, ALEXANDER NEIMAN, Ohio University — We study signal transduction in spontaneously oscillating hair bundles of an auditory hair cell using a computational model. The effects of intrinsic noise from the Brownian motion of hair bundles and from stochastic fluctuations of transduction ion channels as well as periodic fluctuations of the receptor potential are taken into account. The model shows the explosion of a canard trajectory near the Hopf bifurcation. We have found that the system's gain of weak mechanical stimuli can be greatly enhanced when the system operates slightly beyond the Hopf bifurcation, i.e. in the canard region. The gain can also be optimized by tuning the noise intensity.

10:36AM Y9.00014 The co-existence of spirals with multiple rates of rotation JOSEPH TRANQUILLO, Bucknell University — Two findings in homogeneous reaction-diffusion media are that a single spiral may break into multiple spirals and that rapidly rotating spirals push slowly rotating spirals to domain boundaries. These two findings together fail to explain how cardiac tissue can support multiple stable spirals with different periods of rotation. Numerical simulations are presented in which a thin inhomogeneous region forms a functionally protective barrier between spirals rotating at different rates. The only requirement of the insulating region is that it partially block alternating wavefronts from the fast spiral. Parameters of both reaction and diffusion can result in functional insulation and multiple insulating regions can result in the broad frequency spectrum characteristic of cardiac fibrillation. The results suggest that the healthy ventricle, although containing intrinsic inhomogeneities, is functionally connected, while disease may create functionally disconnected regions. This simple mechanism may shed light on why defibrillation and pacing are not always successful, and why some patients are more susceptible to a transition from tachycardia to fibrillation.

**Friday, March 20, 2009 8:00AM - 10:24AM**

Session Y10 DMP: Focus Session: Optical Properties of Nanostructures VI: Artificially Structured Materials
8:00AM Y10.00001 Green’s Functions in Nanoscience1. MURILO L. TIAGO, Oak Ridge National Laboratory — Theoretical nanoscience is a fast growing area in physics. It gains momentum with the recent advances in related areas such as nanodevice design, synthesis and characterization of novel nanostructures, nanoscale imaging and spectroscopy. Several techniques common to quantum chemistry and condensed matter physics have been applied successfully to the modeling of nanoscale structures. In particular, methods based on many-body Green’s functions (MBGF) are becoming more and more popular. One of the reasons for this success is that these methods have predicted several phenomena at nanoscale, for example the peculiar dimensional confinement of excitons in nanostructures. Further advances in quantum transport and exciton dynamics can be foreseen. Moreover, algorithms tailored to confined systems have made calculations of Green’s functions in nanostructures much more manageable [1]. With those algorithms, we were able to investigate the properties of correlated excitations in clusters of semiconductors (CdSe and silicon)[1,2]. We were also able to explain the properties of electronic excitations in fullerene and other organic compounds [1,3]. This talk will present an overview of the current stage of MBGF techniques, discuss the various approximations that have been proposed, and review recent advances.

References:

1Research supported by the Division of Materials Sciences and Engineering BES, U.S. DOE under grant ERKCS77.

8:36AM Y10.00002 First Principles Absorption Spectra of Cu$_n$ ($n = 1$ − 10) Clusters, KOPINJOL BAISHYA, XIANG JUAN, C. IDROBO, SERDAR OGUT, Argonne National Laboratory — First principles optical absorption spectra, obtained within time-dependent density functional theory, for the ground state and low-energy isomers of Cu$_n$ ($n = 1$ − 10) are presented. Overall our theoretical results exhibit good agreement with available experimental data. We analyze the orbital character of the optical excitations as a function of size and energy. Compared to noble metal clusters of Ag and Au in the same size range, we find that Cu clusters have much higher d-electron contribution to low-energy optical excitations.

Supported by DOE Grant No. DE-FG02-03ER15488

8:48AM Y10.00003 ABSTRACT HAS BEEN MOVED TO S1.00259 —

9:00AM Y10.00004 Calculations of second harmonic generation by periodically-structured surfaces, WILLIAM SCHAICH, Physics Department Indiana University — We have done finite-difference time-domain (fdtd) calculations of second harmonic generation (shg) from various surface structures. The periodic structures include pairs of metal strips, split-ring resonators, and fishnets. The nonlinear response is described by a set of parameters that multiply products of linear field components. These fields and the resultant second harmonic radiated fields are found in separate fdtd calculations. The shg spectra do not always correlate well with that seen in linear response.

9:12AM Y10.00005 Optical properties of the Folic Acid/APTMS/TiO$_2$ nanosystems, VOLODYMYR TURKOVSKYI, MICHAEL LEUENBERGER, TALAT RAHMAN, DUY LE, Dept. of Physics and NDSTC, Univ. of Central Florida, Orlando, FL 32816, SUDIPTA SEAL, AMPAC, Univ. of Central Florida, Orlando, FL 32816, SANKU MALLIK, Dept. of Pharmaceutical Sciences, North Dakota State Univ., Fargo, ND 58105, ANDRE GESQUIERE, NSTC, Univ. of Central Florida, Orlando, FL 32816 — Our photoluminescence experiments on folic acid (FA) conjugated nanoparticles of TiO$_2$, CeO$_2$ and SiO$_2$ show great promise for a variety of optoelectronic applications for these materials, in particular in the field of modern molecular photoelectronic devices, since they demonstrate a dramatic increase of the photoemission intensity at wavelengths between 500 to 700 nm when the nanoparticles are coated with the 3-aminopropyltrimethoxylane (APTMS) linker/spacer molecule. We report here results of accompanying time-dependent density-functional theory studies of the FA/APTMS/TiO$_2$ nanosystems by using the B3LYP exchange-correlation potential. We demonstrate that the large increase of the photoemission is due to enhanced optical transitions which involve the intermediate energy levels related to the APTMS states. We present details of the geometric and electronic structure and excited states of our nanosystems and their dependence on the characteristics of the nanoparticle. We discuss possible optoelectronic applications for this effect.

Supported by the Office of BES, Division of Chemical Sciences, Geosciences, and Biosciences, under Contract No. DE-AC-02-06CH11357

9:24AM Y10.00006 Optical Properties and Aging of Gasochromic WO$_3$, RUDRESH GHOSH, University of North Carolina at Chapel Hill, Dept of Physics and Astronomy, MATTHEW B. BAKER, RENE LOPEZ, University of North Carolina at Chapel Hill — WO$_3$ as a possible optical gas sensor has gained increasing importance with H$_2$ becoming a major fuel of the future. This has led to efforts to understand the theoretical and practical aspects of the gasochromic behavior of WO$_3$. WO$_3$ films were fabricated using pulsed laser deposition (PLD). Morphological and stoichiometric ratios of films obtained were observed as functions of deposition parameters. We present the optical constants induced by 2% H$_2$:Ar in WO$_3$ films. This allows us to obtain the limits of the gasochromatic change in comparison to ion injection. It was found using Langmuir’s adsorption equation that at low H$_2$ concentrations a high sensitivity is predicted but the coloration could saturate at 57.9 % of the material’s maximum ion adsorption. Poisoning of the films was also addressed by coating with a permeable polydimethylsiloxane layer. It is shown that gasochromic degradation is prevented thus eliminating common atmospheric gases as possible contaminants. Our studies suggest WO$_3$ thin films as highly sensitive and stable optical hydrogen sensors.

Supported in part by DOE-DE-FG02-07ER15842.

9:36AM Y10.00007 Ab initio Bethe-Salpeter Equation approach for aperiodic materials and core-excitations, H. M. LAWLER, J. VINSON, J.J. REHR, University of Washington, E.L. SHIRLEY, NIST — We have recently developed an interface dubbed AI2NBSE between the Bethe-Salpeter optical spectroscopy code NBSE developed at NIST and the $ab$ initio electronic structure code ABINIT [1]. This interface facilitates first-principles calculations of valence-band dielectric response including excitonic effects in insulating crystals. Here we report on the extension of this interface for calculations of 1) dielectric response in complex nano-scale, disordered, and molecular systems, and 2) core-level UV and x-ray response. For the treatment of complex systems, we discuss issues of cell selection, basis size, and the treatment of the screened electron- hole interaction. For the core level response, we address various strategies including explicit treatments of core and semi-core states with plane waves and the PAW representation.

Franz-Keldysh effect in the interband optical absorption of quantum wires

9:48AM Y10.00008 Franz-Keldysh effect in the interband optical absorption of quantum wires, HAROLD SPECTOR, Illinois Institute of Technology, CONGXIN XIA, Henan Normal University — We present a theoretical calculation of the effect of an electric field applied either parallel or perpendicular to the axis of a rectangular quantum wire on the interband optical absorption. We find that the application of the electric field decreases the optical absorption coefficient for both the parallel and perpendicular to the axis electric field configurations. The absorption is greater when the electric field is along the direction of carrier confinement than when it is along the axis of the wire. This difference is due to the effect of the field on the overlap of the electron and hole wave functions.

10:00AM Y10.00009 Surface Enhanced Raman Spectroscopy (SERS) of pyridine on Pt:1

QINGZHEN HAO, Physics Department, Penn State University, LASSE JENSEN, Chemistry Department, Penn State University, PETER EKLUND, Physics Department, Penn State University — SERS studies were carried out on vertically oriented Pt cylinders patterned on quartz substrates via e-beam lithography. Optical absorption indicates that Localized Surface Plasmon Resonance (LSPR) of the Pt cylinders in the UV region, around 300nm. Discrete Dipole Approximation (DDA) simulation was performed to confirm the position of the substrate’s LSFR and also to map the electric field distribution inside and at the surface of the Pt, which allows us to estimate the Electromagnetic enhancement factor (EF). Experimentally, we demonstrate that the total SERS EF is about 5×10^4 using 514.5nm excitation (far away from the LSFR resonance). Using time-dependent density functional theory we have calculated the off-resonance chemical SERS enhancements of pyridine interacting with small Pt clusters. Our results show that the enhancements are much larger than results obtained for small Ag clusters. We are currently exploring the enhancements for different Pt cluster sizes as well as the importance of charge-transfer excitations. These results will provide detailed insights into the mechanism responsible for the chemical enhancement in SERS.

1This work is supported by NSF NIRT ECS 06-09243.

10:12AM Y10.00010 The Effect of Roughened Metallic Films on Colloidal Quantum Dot Energy Transfer1

CHRISTOPHER FERRI, SOMNATH GHOSH, School of Natural Sciences, University of California, Merced, CA 95344, USA, BRENT RICH, MICHELLE KHINE, School of Engineering, University of California, Merced, CA 95344, USA, SAYANTANI GHOSH, School of Natural Sciences, University of California, Merced, CA 95344, USA — We investigate self-organized, roughened metallic surfaces as a platform for enhanced energy transfer between colloidal Cadmium Selenide (CdSe) quantum dots (QD). Pre-stressed thermoplastic substrates are sputter coated with gold palladium (AuPd) to create thin films. When heated, due to differing coefficients of thermal expansion of the plastic and metal, the AuPd film buckles to form micro- to nano-meter sized structures. QDs deposited on these self-organized metallic structures exhibit changes in their static and dynamic optical characteristics, which include spectral red-shift and multiple recombination decay rates. These observations can be attributed to a combination of enhanced electronic coupling between close-packed QDs and plasmonic coupling between the QD and metallic structures. We then leverage these properties to fabricate controlled, directional structures using this self-organized method which can be utilized as biochemical sensors.

1This work was supported Shrink Technologies Inc, CA.

Friday, March 20, 2009 8:00AM - 10:24AM — Session Y11 DCMP: Superlattices and Nanostructures - Electronic Properties 305

8:00AM Y11.00001 Finding structures with specific properties in complex configurational spaces using multi-target inverse band structure approach1

PAULO PIQUINI, Universidade Federal de Santa Maria, 97105-900, Santa Maria, RS, Brazil, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — The conventional strategy to look for materials with desired properties is to use physical intuition to select some candidates among an enormous number of possibilities. Apart the very special cases, the solutions to these search problems are far from obvious. The inverse band structure (IBS) approach, on the other hand, search for the desired electronic structures (instead of atomic configurations) from the beginning. Here we illustrate the power of this inverse approach by applying it to the simultaneous engineering of multi-target problems, which encompass huge configurational spaces: (i) the search of a specific band gap in the quaternary (In,Ga)(As,Sb) structures (instead of atomic configurations) from the beginning. Here we illustrate the power of this inverse approach by applying it to the simultaneous engineering of multi-target problems, which encompass huge configurational spaces: (i) the search of a specific band gap in the quaternary (In,Ga)(As,Sb) structures, (ii) the stacking sequence of (In,Ga)As/InP superlattices leading to band gaps and strains within the range suitable for thermophotovoltaic applications (b).

(a) P. Piquini, P.A. Graf, and A. Zunger, Phys. Rev. Lett. 100, 186403 (2008);
(b) P. Piquini and A. Zunger, Phys. Rev. B 78, 161302 (2008)

1Funded by DOE-SC-BES-DMS, under contract No. 08GO28308 to NREL.

8:12AM Y11.00002 First-principles studies of structure and electronic level alignment at nanoscale CdSe/CdTe heterojunctions1

SHENYUAN YANG, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Group II-VI semiconductor nanostructured heterojunctions with type-II interfacial band offsets have many potential applications in nanoscale optoelectronics and photovoltaics. A key open question is how the electronic level alignment at nanoscale heterojunctions differs from that at their bulk counterparts, and whether bulk intuition can be used to understand their electronic behavior. We use density functional theory and beyond to study the structure and electronic properties of CdSe/CdTe interfaces in bulk-planar and nanowire form. Both periodic “superlattice” geometries and slabs finite along the surface normal are compared. We compute interface atomic and electronic structure, and for small-diameter nanowires, we discuss the impact of quantum confinement, intrinsic strain, and organic ligand passivation on the electronic properties of the interface. Our results are discussed in the context of recent experiments.

1Prepared at LBNL under U.S. DOE contract DE-AC02-05CH11231.

8:24AM Y11.00003 P-type InSb and InxGa1-xAs quantum wells remotely doped with Be

CHOMANI GASPE, MADHAVIE EDIRISOORIYA, TETSUYA MISHIMA, MICHAEL SANTOS, University Of Oklahoma — CMOS circuits require p-type transistors with high hole mobility, in addition to n-type transistors with high electron mobility. We have observed room-temperature hole mobilities of 100 and 600 cm2/Vs in InxGa1-xAs and InSb quantum wells, respectively. The InxGa1-xAs as wells are remotely doped with Be in InxAl1-xSb barrier layers, and grown on InP substrates. The InSb wells are remotely doped with Be in AlxIn1-xSb barrier layers, and grown on GaAs substrates. We will discuss the effects of strain, structural parameters, and defect density on hole mobility in InSb and InxGa1-xAs quantum wells. In zinc-blend semiconductors, a narrower band gap leads to smaller effective masses for electrons and holes. Strain and confinement increase the energy splitting between holes with light in-plane mass and those with heavy in-plane mass. This work was supported by the NSF Grants DMR-0808086 and DMR-0520550.
8:36AM Y11.00004 Predicted Band Structures of Wurtzite III-V Semiconductors Based on Empirical Pseudopotentials , AMRIT DE, CRAIG PRYOR, Department of Physics and Astronomy,University of Iowa — The electronic properties of III-V semiconductor nanowhiskers present a problem since the nanowhiskers often crystallize in wurtzite (WZ) form while the corresponding bulk materials are zincblende. Using empirical pseudopotentials, including spin-orbit coupling, we have computed the bulk band structures for non-nitride III-V semiconductors grown in WZ form, which may be used for electronic structure calculations of nanowhiskers. The calculations make use of transferable model pseudopotentials fit to the zincblende form. We find that due to the stronger breaking of inversion symmetry in the WZ form, there are larger zero field spin splittings than in the corresponding zincblende materials, making WZ nanowhiskers good candidates for novel spin based devices.

8:48AM Y11.00005 Fundamental properties of TiO$_2$ nanostructures: the effects of the size confinement and the surface coverage , GIOVANNI CANTELE, CNR-INFM-Coherentia, Universita’ di Napoli Federico II., Naples, Italy, AMILCARE IACOMINO, Universita’ di Roma Tre and CNISM, U. di R. Napoli, Naples, Italy, FABIO TRANI, DOMENICO NINNO, Universita’ di Napoli Federico II, Naples, Italy, IVAN MARRI, STEFANO OSSICINI, CNR-INFM S-3, Universita’ di Modena Reggio Emilia, Modena, Italy — The titanium dioxide (TiO$_2$) complexes are widely investigated for their multipurpose capabilities. We discuss here a characterization of anatase TiO$_2$ nanocrystals grown by Buffer Layer Assister Growth (BLAG). Amorphous solid water (ASW) was adsorbed as a buffer layer onto SiO$_2$ perfect bipyramidal morphology and then used this NC as a chain repetition unit in the anatase NW. We studied the size confinement and analyzed the effect of surface coverage by functionalization with simple water-derived adsorbates. We found that the structural reconstruction fit the available experimental data, that the band gap shift depends on the crystallinity and that the hydration is important in stabilizing the nanostructures.

9:00AM Y11.00006 Ion scattering from Au nanoclusters formed by buffer layer assisted growth , SNJEZANA BALAZ, JORY YARMOFF, University of California-Riverside — Ion scattering is used to probe the atomic and electronic structure of Au nanoclusters grown by Buffer Layer Assister Growth (BLAG). Amorphous solid water (ASW) was adsorbed as a buffer layer onto SiO$_2$/Si(111) at liquid nitrogen temperature. Au was then evaporated onto the buffer layer to form nanoclusters. The samples were subsequently annealed to room temperature, causing the water to desorb and the clusters to deposit directly onto the substrate. Time-of-flight (TOF) spectroscopy was used to measure 2 keV $^3$Li$^+$ and $^{39}$K$^+$ ions scattered from Au atoms both at low temperature when the clusters reside atop the buffer layer, and after desorbing the water. Small Au depositions yielded a sharp single scattering peak that indicates single layer structures. Following larger depositions, multiple scattering features were present indicating the formation of multilayer nanoclusters. The neutral fraction of scattered $^3$K$^+$, which provides an indication of the filled quantum states, starts at ~50% for small Au coverages and decreases with further deposition, indicating changes in the quantum state occupancy with cluster size.

9:12AM Y11.00007 Cyclotron Resonance of Two-Dimensional Hole Systems in InSb Quantum Wells , JAMES COKER, R. DOEZEMAA, M. EDIRISORIYIA, T. MISHIMA, MIKE SANTOS, University of Oklahoma, X. PAN, G. SANDERS, C. STANTON, University of Florida, L. TUNG, Y.-J. WANG, NH, University of Florida — We report results on the cyclotron resonance of two-dimensional holes in InSb quantum wells. The samples were grown using molecular beam epitaxy. The two-dimensional holes were generated by doping the InSb with phosphorus. The measurements were made using a four-point probe Hall bar configuration. We observed cyclotron resonance features that were attributed to the two-dimensional holes. The energies of the features were determined using the cyclotron resonance expression. The widths of the channels were varied from a lithographic width of 500 nanometers to 2 micrometers, which suggests that high hole mobilities are possible. At higher fields, we observe separate features for different spin-conserving transitions between neighboring Landau levels. The energies of the features depend on the levels’ spin index and Landau level indices. The energies and intensities are explained by a modified Pidgeon-Brown model that explicitly incorporates pseudomorphic mechanical strain. This work was supported by the NSF under Grants DMR-0808086 and DMR-0520550.

9:24AM Y11.00008 Structural and electronic properties of crystals of thiolate-capped Au nanoparticles doped with donor and acceptor molecules: first-principles calculations1 , RONALDO BATISTA, Universidade Federal de Ouro Preto, JONATHAN MARTINS, HELIO CHACHAM, Universidade Federal de Minas Gerais — Structural and electronic properties of crystals of thiolate-capped Au nanoparticles doped with donor and acceptor molecules: first-principles calculations We perform first-principles calculations for crystals composed of periodic assemblies of Au$_{38}$ nanoparticles that are capped with methyliothiol molecules. We consider fcc structures, consistent with recent experimental results [1]. We also consider that the nanoparticle crystals can be doped with either donor (tetrabutylammonium) or acceptor (hexafluorophosphate) molecules, also consistent with recent experiments [2]. We find that the most stable positions of the dopant molecules are located near the nanoparticle surface and that the most interesting changes occur when the dopant molecules are in the center of the nanoparticle. When the concentration of dopants is increased, the stability of the crystal decreases, consistent with recent experiments [2]. Above that critical concentration, a new regime is observed due to a partial order in the dopant molecules. We also consider that the nanoparticle crystals can be doped with either donor (tetrabutylammonium) or acceptor (hexafluorophosphate) molecules, also consistent with recent experiments [2]. We find that the most stable positions of the dopant molecules are located near the nanoparticle surface and that the most interesting changes occur when the dopant molecules are in the center of the nanoparticle. When the concentration of dopants is increased, the stability of the crystal decreases, consistent with recent experiments [2]. Above that critical concentration, a new regime is observed due to a partial order in the dopant molecules. These features are reproduced by a simple capacitive model for the crystal. [1] Abecassis et al. Phys. Rev. Lett. 100, 115504 (2008) [2] Boettcher S. W. et al. Nature Mater. 6, 592-596 (2007).

1CNPq, Fapemig and Instituto do Milhio de Nanociencias

9:36AM Y11.00009 Interaction effects in conductance of quasi-1D channels formed from Al-GaAs/GaAs 2DEG: Crossover from weakly-disordered Fermi liquid to Luttinger liquid1 , MATTHEW BELL, ANDREI SERGEEV, JONATHAN BIRD, VLADIMIR MITIN, ALEKSANDR VEREVKIN, University at Buffalo — We investigated the conductance of a long and narrow high-mobility channel and observed weakly-disordered multi-channel Fermi liquid [1] to Luttinger liquid with decreasing channel width to ~100nm. Quasi-one-dimensional channels were formed from an AlGaAs/GaAs heterostructure using the split-gate technique. The lengths of the channels were 100 μm. The width of the channels were varied from a lithographic width of 500 nm to ~50 nm by applying negative bias to the split-gate. The effective electron concentration and the channel widths were evaluated from magnetoresistance measurements. In the range of channel widths 500 - 100 nm, at temperatures 1-10 K we clearly observe the logarithmic temperature dependences of the conductance. These dependences are adequately explained by effects of electron-electron interaction in weakly-disordered quasi-one dimensional (with respect to the interaction) Fermi liquid [1]. When the width further decreases, the logarithmic dependences change to power-law dependences, which are typical for Luttinger liquid. This crossover takes place when the channel width corresponds to 2-3 one-dimensional subbands. [1] Sergeev et al., Phys. Rev. B. 69, 075310 (2004).

1This research was supported by grants from NYSTAR and AFOSR

9:48AM Y11.00010 Giant Orbital Paramagnetism in Nanometer Scale 2DEG Strips , MICHAEL HARRISON, Michigan State University — An elementary calculation shows that Landau diamagnetism becomes significantly altered and very large paramagnetic effects emerge at low temperatures when the channels are penetrated by a perpendicular applied magnetic field and bounded by a parabolic potential, such as may arise from negative voltage applied to a split gate. These novel results are described by an expression which manifests the total system magnetization as a difference between evolved orbital paramagnetism and altered diamagnetism. These predicted effects correspond to drift motion of electrons parallel to the strip length arising from Landau eigenstates that are non-degenerate in the combined presence of a perpendicular applied magnetic field and electric fields associated with a confining parabolic potential. A new heterostructured magnetic material based on orbital electronic motion in 2DEG strips is proposed.
10:00AM Y11.00011 Excitonic condensation with different pairing symmetries in double quantum wells, CHRISTOPHER JAMEL, Indiana University-Purdue University Indianapolis — Double quantum wells with one containing electrons and the other containing holes as carriers are a promising candidate for condensation of dipolar excitons with lifetime much larger than lifetime of excitons in bulk quantum wells. When the inter-well distance is comparable to the interparticle distance within a single well, $d \leq r_{dip}$, inter-well coherence is expected to lead to an excited state condensation. We explore the ground state of a balanced system as a function of inter-well distance and order parameter dispersion with different pairing symmetries. We obtain the quasiparticle density of states in each case. These results lay the ground work for mean-field study of excitonic condensate states with spontaneously broken translational symmetry.

10:12AM Y11.00012 Coulomb Blockade in a Field Emitting Freely Suspended Island, CHULKI KIM, Physics, University of Wisconsin-Madison, HYUN S. KIM, Electrical & Computer Engineering, University of Wisconsin-Madison, HUA QIN, Suzhou Institute of Nano Tech and NanoBionics, ROBERT H. BLICK, Electrical & Computer Engineering, University of Wisconsin-Madison — We observe staircase current-voltage characteristics from an isolated nanomechanical island. The island is fixed by CF$_3$ connections, which makes the structure suspended 1m above SiO$_2$. The noteworthy difference to the “orthodox” single electron transistors is the fact that we observe Coulomb blockade in conjunction with field emission. We can trace and reproduce the transition from staircase to high bias regime. A theoretical model based on field emission current reproduces the experimental data. The full profile of the current-voltage measurement shows the transition from Coulomb staircase current to island field emission current.

Friday, March 20, 2009 8:00AM - 11:00AM —
Session Y12 DCMP DMP: Electronic and Lattice Properties, Including Quantum Size Effects

8:00AM Y12.00001 Bi(114): A quasi one-dimensional metal with strong spin-orbit splitting, PH. HOFMANN, University of Aarhus, DK, J.W. WELLS, University of Aarhus, DK and University of Science and Technology, Trondheim, N, H. DIL, P. MEIER, University Zurich-Irchen and SLS, PSI, CH, J. LOBO-CHECA, University Zurich-Irchen and SLS, PSI and Basel University, CH, V.N. PETROV, St. Petersburg Technical University, RU, J. OSTERWALDER, University Zurich-Irchen, CH, M.M. UGEDA, Free University Berlin, D and University Autonoma de Madrid, ES, I. FERNANDEZ-TORRENTE, J.I. PASCUAL, Free University Berlin, D, E. Rienks, M.F. Jensen, University of Aarhus, DK — The (114) vicinal surface of the semimetal Bi is found to support a quasi one-dimensional, metallic surface state. As required by symmetry, the state is degenerate along the $\Gamma - X$ line of the surface Brillouin zone with a binding energy of $\sim$100 meV. In the $\Gamma - X$ direction the degeneracy is lifted by the strong spin-orbit interaction, as directly shown by spin-resolved photoemission. This results in a Fermi surface consisting of two closely separated, parallel lines of opposite spin direction. We discuss these findings in the light of the recently discovered topological stability of surface states on Bi$_2$S$_3$ topological insulators.

8:12AM Y12.00002 Plasmon Resonances in Ultrathin Magnesium Films, MUSTAFA M. OZER, ORNL Oak Ridge TN, EUN JU MOON, Univ Tennessee Knoxville TN, ADOLFO G. EGUILUZ, HANNO H. WEITERING, Univ Tennessee Knoxville TN & ORNL Oak Ridge TN — Low temperature growth of Mg on Si(111) results in the formation of atomically smooth thin films with precisely controlled film thickness. We employed x-ray photoelectron spectroscopy to monitor the evolution of a sharp shake-up satellite in the Mg 1s core level as a function of the film thickness. For films with thicknesses between five and five atomic layers the energy position of this peak is inversely proportional to the square of the film thickness. These results are consistent with the existence of quantized plasmons, which we interpret on the basis of theoretical (hydrodynamics and RPA) descriptions of the density-response function. We demonstrate that the observed loss feature corresponds to the $n = 1$ antisymmetric normal mode of the thin film, consistent with the fact that in the ultrathin film limit the symmetric plasmons have vanished spectral weight - a striking manifestation of the role of size quantization on plasmon resonances in precisely controlled nanostructures.

8:24AM Y12.00003 Structural analysis of the surface of bilayered ruthenate Sr$_3$Ru$_2$O$_7$, BIAO HU, University of Tennessee, Knoxville, TN, D. MANDRUS, A.P. LI, M.H. PAN, Oak Ridge National Laboratory, Oak Ridge, TN, SHUHENG PAN, University of Houston, Houston TX, V. Nascimento, E.W. PLUMMER, Louisiana State University, Baton Rouge, LA, R. JIN, Louisiana State University, Baton Rouge, LA and Oak Ridge National Laboratory, Oak Ridge, TN — The bilayered ruthenate Sr$_3$Ru$_2$O$_7$ exhibits interesting structural properties. For example, in the bulk the in-plane lattice parameter $a$ expands while the out-of-plane lattice parameter $c$ contracts as temperature decreases, accompanied by a rotation of RuO$_6$ octahedra. Remarkably, the broken translational symmetry at the surface causes a tilt of RuO$_6$ octahedra. The Low Energy Electron Diffraction (LEED) $I - V$ analysis shows that the tilt angle of RuO$_6$ is temperature dependent and hysteretic. The correlation between RuO$_6$ tilt at the surface, the surface thermal expansion, and the electrical properties were investigated using Scanning Tunneling Microscopy, (LEED)-$I - V$, and Scanning Electron Microscopy.

8:36AM Y12.00004 Interface-Induced Complex Electronic Interference Structures in Ag Films on Ge(111), TAI CHIANG, YANG LIU, NATHAN SPEER, University of Illinois, Urbana-Champaign, SHU TANG, National Tsing Hua University, TOM MILLER, University of Illinois, Urbana-Champaign, UNIVERSITY OF ILLINOIS, Urbana-Champaign TEAM — We have mapped the electronic structure of atomically-uniform films of Ag grown on Ge(111) by angle-resolved photoemission. Cuts in momentum space at constant energies near the Fermi surface reveal intricate patterns resembling interfering waves emanating from multiple centers. The measured dispersion relations exhibit zigzag patterns with multiple energy gaps. These features are attributed to the mixing of electronic standing waves by the Ag-Ge interface potential, as confirmed by the observed pattern symmetry and by an experimentally deduced interaction strength that scales as the inverse film thickness.

8:48AM Y12.00005 Influence of quantum well states on the formation of surface Au/Pb alloy in Pb/Si(111) quantum thin films, JUNGDAE KIM, SHENGYONG QIN, ALEXANDER KHAJETTOORIANS, University of Texas at Austin, WENGIANG ZHU, ZHENYU ZHANG, The University of Texas, Oak Ridge National Laboratory, CHIH-KANG SHIH, University of Texas at Austin — The thickness dependence of Au/Pb alloy formation on thin Pb quantum films is studied using in-situ low temperature STM/S. Sub-monolayer Au was deposited on thin Pb films on Si(111) substrates. When deposition is carried out at a substrate temperature close to room temperature, it is found that local Au/Pb surface alloys are formed in the form of nano-islands, with preferential formation probability at certain thicknesses. STS data shows this is directly related to quantum well states (QWS) of underlying Pb mesas. When the growth is carried out at low temperature (~80K), the alloy formation probability doesn't show strong thickness preference, but QWS has still strong influence on the nature of the Au/Pb alloy. Two types of Au/Pb alloy nano-islands are formed with quite different electronic properties.

1 NSF-FRG DMR-0606485
9:00AM Y12.00006 Coherent quantum-well electronic structure in bimetallic Pb/Ag films prepared on Si(111). MATTHEW BRINKLEY, Univ of Illinois at Urbana-Champaign, YANG LIU, NATHAN SPEER, THOMAS MILLER, TAI-CHANG CHIANG, UIUC — Angle-resolved photoemission is employed to investigate the electronic structure of Pb films of various thicknesses grown on atomically uniform Ag(111) films. The Ag films, which were deposited on Si(111) substrates, host fully confined electrons at energies within the absolute gap of Si and partially confined electrons outside. The question is: What is the electronic structure of the Pb films prepared over the Ag films? Our results reveal that the quantized electronic structure of the Ag films can be detected for Pb overlays with thicknesses much larger than the photoemission escape depth. Comprehensive simulations have been performed and are in agreement with the experimental results. This study reveals a strong coherent coupling of the Ag and Pb electronic structures despite the incommensurate Ag/Pb interface.

9:12AM Y12.00007 Pseudogap Mediated by Quantum-Size Effects in Lead Islands, KEDONG WANG, XIEQIU ZHANG, Chinese University of Hong Kong, M.M.T. LOY, Hong Kong University of Science and Technology, T.-C. CHIANG, University of Illinois at Urbana-Champaign, XUDONG XIAO, Chinese University of Hong Kong — Quantum confinement effects in both metallic and semiconducting materials are subjects of intense prevailing interest. For thin films and islands of Pb grown on semiconductor surface, quantum well states have been clearly identified and their consequences in growth, thermal stability, and superconductivity have been well studied. In this talk, we will present scanning tunneling spectroscopy measurement results of Pb islands on Si(111) at high energy resolution that reveal a novel pseudogap, or a pseudopeak in special cases, around the Fermi level in addition to the usual quantum well states. These gap or peak features persist to temperatures as high as ~80 K and are uniquely related to the quantum well nanostructure of the Pb islands. A systematic analysis indicates that electron-phonon scattering is responsible for the observed electronic structure. The behavior of the pseudogap has a strong resemblance to that of the pseudogap in high temperature superconductors and certain connections may be speculated.

9:24AM Y12.00008 Quantized Electronic Structure and Growth of Pb Films on Highly Oriented Pyrolytic Graphite, YANG LIU, UIUC, JENS PAGGEL, Continental Automotive GmbH, MARY UPTON, Argonne National Lab, TOM MILLER, TAI CHIANG, UIUC, UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN TEAM — We have measured the electronic structure of thin Pb films grown on highly oriented pyrolytic graphite (HOPG) by angle-resolved photoemission spectroscopy. Quantum well states (QWS) corresponding to confined Pb valence electrons are observed. Although the films are rough, the thickness distribution is sufficiently narrow to allow a unique assignment for each QWS peak in terms of a quantum number and the exact film thickness in atomic layers. The even film thicknesses are found to be much more prevalent than the odd film thicknesses. These results are consistent with an available first-principles calculation of the surface energies of freestanding films; an implication is that the interaction between the Pb film and the HOPG substrate is weak. The effective masses of QWS at the surface zone center agree well with the results calculated from the bulk Pb band structure, in sharp contrast to the strongly enhanced or anomalous effective masses in Pb films grown on Si(111) as reported previously. This finding indicates that the anomalous effective masses in Pb/Si(111) are not caused by increased electron correlation effects in a confined geometry, but rather attributable to a strong interfacial interaction between the QWS and the substrate electronic structure.

9:36AM Y12.00009 Quantum stability and superconductive properties of atomically smooth ultrathin alloy films of thermodynamically immiscible metal elements1, EUN JU MOON, Univ Tennessee, Knoxville, MUSTAFA M. OZER, ORNL, JAMES R. THOMPSON, HANNO H. WEITERING, Univ Tennessee, Knoxville, and ORNL — Pb and Gd are immiscible in bulk form. However, atomically smooth ultrathin films of Pb1−xGdx (x=0.06) can be stabilized on a Si(111)7x7 substrate through the quantum size effect. The quantum stability and superconductive properties of these films were investigated using STM, XPS, and SQUID magnetometry measurements. Quantum stabilized growth defects, consisting of deep holes extending to the film-substrate interface, act as pinning centers for vortices in the superconducting state. The pinning centers support an extraordinarily robust critical state with critical current densities in excess of 3 MA/cm2 in 10 monolayer thick films. Anomalies in the dc magnetization and ac magnetic response below 2.5-3.5 K indicate a reduction of the flux pinning below these temperatures, which we attribute to the nature of the holes (deep holes as opposed to blind holes in pure Pb films). The present study highlights the possibility of growing new alloys beyond the solid solubility limit and controlling critical state properties in the quantum regime.

1Research at ORNL sponsored by DOE, Div of Mat Sci Eng.

9:48AM Y12.00010 First-principles study of SiOx/SiC(0001) surface insulating layer, YASUNOBU ANDO, University of Tokyo, KAZUTO AKAGI, WPI-AMR, Tohoku University, SHINJI TSUNEYUKI, University of Tokyo, TETSUROH SHIRASAWA, ISSP, University of Tokyo, HIROSHI TOCHIHARA, Kyushu University, MASAHIRO SATO, Kyushu University, HIROYUKI OHTOMO, Kyushu University, MASAHIRO SATO, Kyushu University, MASAHIRO SATO, Kyushu University, MASAHIRO SATO, Kyushu University — We have calculated by first-principles methods self-consistently the electronic structure of a SiC/SiO2/SiC heterostructure grown on SiC(0001) substrate. The SiO2 layer is terminated by a hydrogen atom, which acts as the source of the charge carriers. The charge carrier density and spatial distribution are not fully understood. In presentation, first-principles study for establishing the fundamental property of the charge carrier in the intrinsic n-type LaAlO3/SrTiO3 interface is introduced. To this end, large models systems including up to 20 layers of SrTiO3 and 1–10 layers of LaAlO3 are employed. The charge carrier is observed within the LaAlO3 layers, with a density as high as 10^18 cm^-3.

10:00AM Y12.00011 Electronic structures of intrinsic n-type SrTiO3−xLaAlO3 interface: density and spatial distribution of free carriers, WON-JOON SON, EUNAE CHOI, SEUNGWU HAN, Ewha Womans University — The seminal paper by Ohtomo and Hwang reporting the unexpected conductivity when two perovskite insulators, SrTiO3 and LaAlO3, formed an atomically abrupt interface along [001] direction, has aroused immense interest on the origin of the conductivity. While it is widely accepted that the intrinsic n-type interface is conducting, the carrier density and its spatial distribution are not fully understood. In presentation, first-principles study for establishing the fundamental property of the charge carrier in the intrinsic n-type LaAlO3/SrTiO3 interface is introduced. To this end, large models systems including up to 20 layers of SrTiO3 and 1–10 layers of LaAlO3 are employed. The charge carrier is observed when LaAlO3 is larger than 3 unit cells and confounded to 5 electrons per unit cell. It is also found that the charge carriers transferred from SrTiO3 surface are mostly localized within a few layers from the interface. Furthermore, the electronic states are quantized at the interface with different localization widths, which is similar to electrons in a wedge potential. The carrier density contributed by the interface-localized state shows a good agreement with the experiment.

10:12AM Y12.00012 ABSTRACT WITHDRAWN —
10:24AM Y12.00013 Positron states and annihilation characteristics at the reconstructed (100) and (111) surfaces of Si with adsorbed hydrogen and oxygen. N.G. FAZLEEV, W.B. MADDOX, A.H. WEISS, Department of Physics, University of Texas at Arlington — We present results of theoretical studies of positron surface states, work functions and annihilation characteristics at the reconstructed (100) and (111) surfaces of Si with adsorbed hydrogen and oxygen. Calculations are performed taking into account geometrically optimized surface structures using a modified superimposed-atom method, and employing the corrugated-mirror model in a full three-dimensional geometry. The effects of adsorption of hydrogen and oxygen on the positron binding energy at the reconstructed (100) and (111) surfaces of Si and the positron work function are explored. The positron surface-state annihilation characteristics are computed for different hydrogen and oxygen coverages of both reconstructed surfaces of Si. The obtained results predict attenuation of the Si positron-annihilation-induced Auger electron signal intensity with the increase of the hydrogen and oxygen coverage consistent with experimental data. These studies confirm that positron-annihilation-induced Auger electron spectroscopy can be used to study changes in the properties of semiconductor surfaces due to the presence of adsorbed hydrogen and oxygen.

10:36AM Y12.00014 Fabrication and transport measurement of periodic wavy structures of Si/SiGe nanomembranes, MINRUI YU, ROBERT BLICK, ARNOLD KIEFER, DON SAVAGE, MAX LAGALLY — We demonstrate fabrication of completely under-etched Hall-bars made from Si/SiGe nanomembranes with a highly doped SiGe layer. The sample material is epitaxially grown by chemical vapor deposition (CVD) on silicon-on-insulator (SOI) wafers. Hall-bars are defined by optical photolithography and etched by reactive ion etching (RIE). They are then completely released from the substrate through hydrogen fluoride (HF) vapor etching. The lattice mismatch between silicon (Si) and germanium (Ge) generates an initial strain inside the material, which tends to recover once the sacrificial oxide layer is removed. This combined with carefully designed geometric constraints causes the structures to buckle and generate periodic wavy patterns after releasing and rebonding to the wafer surface. We study the magneto-transport at both room and low temperatures, with and without light illumination. Our results show the effect of strain on band structure and electron mobility. This will further the understanding of mechanically modulated electron transport.

10:48AM Y12.00015 Electron accumulation on bare and hydrogenated indium nitride surfaces, BRIAN THOMS, RUDRA BHATTA, ANANTA ACHARYA, MUSTAFA ALEVLI, NIKOLAUS DIETZ, Georgia State University, DEPARTMENT OF PHYSICS & ASTRONOMY TEAM — Electron accumulation layers which affect device and contact properties have been reported on several semiconductor surfaces such as InAs, InN, and CdO. Adsorbates have been shown to affect the electron density on InAs surfaces, however, surface termination effects for InN have not been determined. In this work surface-sensitive electron spectroscopic techniques are used to study both the electron accumulation layer and the surface structure on N-polar InN. High resolution electron energy loss spectroscopy (HREELS) has been used to characterize the surface electron accumulation by observing changes in the energy of the conduction band plasmon loss with variations in incident electron energy. In addition, HREELS along with low energy electron diffraction and Auger electron spectroscopy allow characterization of the surface structure and bonding. By this method it is shown that both hydrogen-terminated and bare N-polar InN surfaces exhibit electron accumulation. These results indicate that surface electron accumulation on InN is not due to indium-indium bonding and is not substantially affected by the presence or absence of surface hydrogen, but may instead be intrinsic to the N-polar InN surface. The effects of other adsorbates will also be discussed.

Session Y13 DCOMP: General Theoretical and Computational Methods 309

8:00AM Y13.00001 A global EMC/FDTD simulation tool for modeling THz wave interaction with conductive media, K. J. WILLIS, S. C. HAGNESS, I. KNEZEVIC, University of Wisconsin - Madison — We present a computational tool for modeling the interaction between THz electromagnetic waves and conductive media. By coupling the ensemble Monte Carlo (EMC) simulator of carrier dynamics and the finite-difference time-domain (FDTD) solver of Maxwell's equations, we have developed a robust and versatile global simulator that can be applied to the fields of linear algebras, FFT, and others. We have experienced that one-dimensional CUFFT ver1.1 (GPU-FFT) is eight times faster than FFTW for single-precision case. We implement the GPU-FFT into our in-house first principles planewave code, in which the hot spot is the FFT routine. We will present the fields of linear algebras, FFT, and others. We have experienced that one-dimensional CUFFT ver1.1 (GPU-FFT) is eight times faster than FFTW for single-precision case. We implement the GPU-FFT into our in-house first principles planewave code, in which the hot spot is the FFT routine. We will present the performance of the implementation.

8:12AM Y13.00002 GPU Based Acceleration of First Principles Calculations, HIDEKAZU TOMONO, Meiji University, JAPAN, TOSHIKAI IITAKA, RIKEN, KAZUO TSUMURAYA, Meiji University, JAPAN — The saturation of the acceleration using the silicon devices has required the parallel computing using multiple CPU's (central processing units). The parallel computing has been widely used in the field of the high-performance computing. On the other hand, graphics processing units (GPU's) were designed to accelerate graphic applications in 1978. NVIDIA Co. began to provide CUDA for C-language users to manipulate the GPU's in 2007. They applied it to computational fluid dynamics, medical real time simulation and astronomical N-body problem among others. This is the GPGPU (general-purpose computation on GPU's), which is faster in operation than CPU in the fields of linear algebras, FFT, and others. We have experienced that one-dimensional CUFFT ver1.1 (GPU-FFT) is eight times faster than FFTW for single-precision case. We implement the GPU-FFT into our in-house first principles planewave code, in which the hot spot is the FFT routine. We will present the performance of the implementation.

8:24AM Y13.00003 Saturation effects in dispersion interactions, BO E. SERNELIUS, Linköping University — The interest in Casimir interactions has been very strong during the last decade. This increase in interest was spurred by the torsion pendulum experiment by Lamoreaux which produced results with good enough accuracy for the comparison between theory and experiment to be feasible. Theory and experiment agree quite well for low temperatures. However at room temperature, where most experiments are performed there are serious deviations. Each new experiment has lead to new puzzling discrepancies between theory and experiment. Theorists have been forced to resort to phenomenological approaches to the problems, with new prescriptions for each new experiment. Here we address three experiments: Casimir pressure between a gold sphere and a gold plate; Casimir force between a gold sphere and a laser excited silicon membrane; Casimir force between a Rub atom and a fused silica wall. In all these different experiments we show that inclusion of saturation effects makes the discrepancies go away.

8:36AM Y13.00004 Symmetries of non-relativistic quantum-mechanical Hamiltonian, BOJAN TUNGUZ, Wabash College — In non-relativistic quantum mechanics the most fundamental invariance group of the Hamiltonian is the Galilean group of transformations: the group spatial and temporal translations and rotations. The quantum-mechanical wave functions in that view belong to an infinite-dimensional representation of the Galilean group, and the generators are represented with first-order differential operators. In this work we look at all the higher order differential operators that commute with the Hamiltonian and construct the most general group that leaves the Hamiltonian invariant. We show how the Galilean group fits within this group, and we show how the interaction terms break the symmetry of the free-particle Hamiltonian. We argue that the interpretation of the Hamiltonian in terms of individual interacting particles is the consequence of this broken symmetry.
8:48AM Y13.00005 Planck’s High Temperature Catastrophe in Observational Astronomy:- (NASA proves Planck wrong) , CLARENCE A. GALL, Universidad del Zulia, Venezuela — Planck’s black body radiation law 

\[ I_B = \frac{2 \pi^2 \hbar^2 c^2}{\lambda^5 (e^{\lambda/\kappa} - 1)} \]

predicts that a hotter body (higher \( T \)) should always emit more intensely than a colder body (lower \( T \)) throughout the entire EMR spectrum. However, space age infrared astronomy contradicts this prediction! It is now known that as observation moves from the visible to the near-, mid- and far infrared; increasingly cold celestial objects come into view while hotter ones fade and disappear (http://coolcosmos.ipac.caltech.edu/cosmic_classroom/ir_tutorials.html). Were Planck’s law valid, the hottest stars would never disappear; and colder objects would not be detected. This can only be described as a high temperature catastrophe (APS, April Meeting 2008; H12.3, St Louis, MO) for Planck’s law! On the other hand, Gall’s black body radiation law

\[ I_B = \frac{\sigma T^4}{\lambda^5} \]

(http://sites.google.com/site/purefieldphysics) predicts that as wavelength increases, there is a crossover point above which a colder object will emit more intensely than a hotter one. Hence colder objects will appear and hotter ones will eventually disappear from view. The crossover point for black bodies at 6000K and 100K is 12.066 microns. These calculations with Gall’s law are in overall agreement with observational infrared astronomy.

9:00AM Y13.00006 Expressing n dimensions as n-1. JOHN LAUBENSTEIN, IWP Research Center — The IWP Scale Metrics team has explored a different conceptualization of multiple dimensions through a model expressing n dimensions as \( n-1 \). This is achieved by aligning time and a spatial dimension along the same orientation. We have shown that time and distance along the same axis in combination with a scalar is equivalent to two orthogonal dimensions. Scale Metrics is simply a different conceptualization of multi-dimension. However, it requires a change in the modeling of gravitation since time is no longer considered to be orthogonal to the three spatial dimensions. A model for Scale Metrics gravity has been developed and in the process a quantum theory of gravitation emerges. Why entertain IWP Scale Metrics? Because the Standard Model has not been successful in the unification of GR with QT. A new model of gravitation built on a foundation of quantum concepts (as opposed to a quantum fix to an inherently classical geometric theory) may be the key to understanding the universal stage for the unification of gravitation with quantum theory. Further, since Scale Metrics provides nothing more than a different way to conceptualize multiple dimensions in a manner that is equivalent to 4 vectors – it replaces nothing, but rather serves only to complement past and current achievements while providing a new view of quantum gravitation.

9:12AM Y13.00007 The mass, energy, space and time system theory-MEST- the theory of relativity and the quantum mechanics. DAYONG CAO, Beijing Natural Providence Science & Tech — Things have their own physical system of mass, energy, space and time of themselves. (The MEST for short thereafter) So we can use it to unite both the physical system of any thing. There are the transmutation between space-time and mass-energy. There are the conservation of space-time and mass-energy. The uf force like the gravitation is from space-time, the down force like repulsion is from mass-energy. So there are the positive and negative curvature. We need to develop the theory of relativity and get the new equation. By using the mass-energy wave equation, deduce the new uncertainty principle, uncertainty and probability can not be divided. New wave wave equation are being put forward. The quantum mechanics is the mass and energy theory of relativity; the theory of relativity is the space and time theory of relativity. MEST can unite both them.

9:24AM Y13.00008 Is Sound a Property of Space or Vacuum? , VENKATA CHAGANTI, Department of Physics, University of Texas, El Paso — Absolutist regards SPACE as an entity in its own right with properties of its own. Further more, relationists, scientists and laymen attribute many different sorts of properties to SPACE. In fact, we are able to distinguish every material from the other by its properties. We all know that SPACE is attributed by some of the properties listed below. 1. Electromagnetic Properties like permittivity and permeability. 2. Empty SPACE is a poor conductor. 3. Empty SPACE is transparent. 4. SPACE is penetrable by any particle / material. 5. SPACE is incapable of action. 6. SPACE is immovable. 7. SPACE is infinite. 8. SPACE is isotropic. 9. All bodies are place in SPACE. 10. SPACE is Isotropic. And many more properties can be made quite precise without any reference to an embedding space surrounding the SPACE of interest. SPACE as a physical object only makes sense if it can be detected, or if it can exert physical influences. Does the motion of an object through SPACE lead to detectable effects? Can SPACE act on a moving body in the way that the sea acts on a moving fish? In this paper an attempt is made to show that SPACE is indeed like any other medium / material and also SOUND is its property. Statistical Mechanics is used as a tool.

9:36AM Y13.00009 New Generally Covariant Generalization of the Dirac Equation Not Requiring Gauges , DAVID MAKER, mda — We introduce a new pde \( \left( \sum_{\mu} \sqrt{\gamma_{\mu} \gamma_5} \partial / \partial x_{\mu} \nu = 0 \right) \) with symmetrically diagonalized \( \kappa_\nu = 1 \rightarrow H \)

\[ \frac{1}{\kappa \nu} \] giving it common covariance. If \( \kappa_\nu = 2 \) this new pde reduces to the standard Dirac equation as \( \nu \rightarrow \infty \). Next we solve this equation directly using separation of variables (e.g., 2P, 25, 15 terms). Note metric time component \( \kappa_\nu = 0 \) at \( \nu \rightarrow H \) and so clocks slow down with baryon stability the result. Note also that near \( \nu \rightarrow H \) the 2P state for this new Dirac equation gives a circumtrifoulum, 3 lobe shape; so this ONE charge (so don’t need color to guarantee this) spends \( 1/3 \) of its time in each lobe (fractionally charged lobes), the lobe structure is locked into the center of mass (asymptotic freedom), there are six 2P states (corresponding to the 6 flavors); the P wave scattering gives the jets, all these properties together constituting the main properties of quarks! without invoking the many free parameters, gauge conditions of QCD. Also the 25L/1 \( \rightarrow \) the tauon and the 15L/1 \( \rightarrow \) the muon here. The 5S of this new pde gives the \( W \) and \( Z \) as resonances and does not require renormalization in free parameters. Thus we get nuclear, weak and E&M or phenomenology as one step solutions of this new pde, not requiring the standard method’s pathology of adhoc assumptions such as gauges and counterterms, 19 free parameters (you can vary any way you want) that have confused, blocked the progress of theoretical physics for the past 30 years.

9:48AM Y13.00010 The darkness of mere being: DM and DE explained , JAMES BEICHLER, Retired — In previous APS meetings, I have presented a geometrical explanation of Dark Matter and Dark Energy that makes testable predictions and is thus completely falsifiable. The theory is based on a macroscopically extended fourth dimension of space that yields a five-dimensional space-time structure. In this structure, the four-dimensional space-time of relativity is extrinsically curved in the higher spatial dimension. Dark Matter is curvature in the higher dimension that is not directly associated with local matter, but instead results from an interaction between local matter or curvature and the global curvature due to all matter in the universe. Criticisms that the theory was not mathematical have now been overcome and a simple algebraic formula that corresponds to the geometry of the four-dimensional structure of space has been derived. The algebraic formula appears to be Newtonian, but it implies a five-dimensional unified field structure such as that developed by Kaluza in 1921 and extended by Einstein and his colleagues in the late 1930s. The new equation also shows how gravity can be quantized on the basis of relativity without hypothesizing the discrete nature of matter, i.e., the existence of specific “particles” of gravity, inherent in quantum mechanics, the Standard Model and other quantum models.

10:00AM Y13.00011 Charged Particles are Preventing from Moving Faster than the Speed of Light by Light Itself , RANDY WAYNE, Department of Plant Biology, Cornell University, Ithaca, NY 14853 — Many problems in classical mechanics are solved by assuming that friction is negligible. At velocities close to the speed of light, however, friction is never negligible as a consequence of the dilatant optical molasses that results from the temperature-dependent blackbody distribution of photons. A body moving at relativistic velocities experiences the blackbody radiation as being Doppler shifted. This adds a nonlinear velocity-dependent component of friction. By accounting for this thermodynamic friction, I have obtained an equation of motion that is applicable for modeling the movement of particles at relativistic velocities. While the predictions of the opto-mechanical model are qualitatively consistent with the predictions of the Theory of Special Relativity in terms of the nonlinear relationship between force and acceleration, there are quantitative and testable differences.
10:12AM Y13.00012 Why So Many More Americans Die in Fires. LAWRENCE CRANBERG, Texas Fireframe Co. — “Why So Many More Americans Die in Fires” is the headline on Page 3 of The New York Times’ full-page story on December 22, 1991, by D. G. McNeil, Jr. — It is a partial report based on personal experience with domestic fire making for thermal comfort since 1975 (1) and a published claim (2) of unique safety benefits. The McNeil report attributes the problem to “A Case of Bad Attitude” and “A Reliance on Technology.” That implies a “bad attitude” on the part of technologists – a conclusion consistent with this technologist’s thirty-five years of experience with fellow technologists, who has found “buck-passing” the favorite recourse of technologists in the highest places in government even though, as McNeil has written, “Many children never wake up. Smoke or toxic gases overcome them as they sleep. When fire fighters lift them, their imprints remain.” Regrettably, in this author’s experience, the courts have also displayed a “bad attitude” where “life and death issues” have been pleaded. 1. L. Cranberg, Slot Flame Stability with Hohlraum Radiation Pattern, BAPS, Series II, Vol. 20, No. 9, Sept., 1978. 2. L. Cranberg, Fireplace Firesafety, Fire Journal, Letter, May/June, 1987.

10:24AM Y13.00013 A new Virtual Crystal Approximation approach, ROBERTA POLONI, ICMAB-CSIC, Campus UAB E-08193 Bellaterra, Barcelona (Spain) — It is well known that the virtual crystal approximation (VCA) provides an efficient method for studying disordered alloys and solid solutions by first-principles. Although several studies have reported VCA results regarding stability issues by using energetic considerations, here we propose a new approach based on alternative structural indicators. The reason for this is that it is still not clear whether energy comparisons for different virtual compositions are trustworthy. Our non-fully-predictive scheme makes use of some experimental information in order address structural problems like atomic ordering and/or partial occupation at some site. We look at different figures of merit (energy derivatives), depending on the amount of experimental information taken into account, and we minimize them with respect to different possible structural configurations. By applying our approach to a wide number of well known systems (oxinitrides, borocarides, perovskites, etc.) we have been able to reproduce the experimental structure in all cases.

Friday, March 20, 2009 8:00AM - 9:48AM — Session Y14 DFD: Nonequilibrium and Templated Assembly 315

8:00AM Y14.00001 Speeding up the understanding of Vertical Deposition of Diluted Colloids1, WENCESLAO GONZÁLEZ-VIÑAS, MAXIMILIANO GIULIANI2, MOORTHI PICHUMAN3, University of Navarra — We measured the speed of contact line in vertical deposition of diluted micron sized polymeric colloids. We correlated these results with the obtained morphologies for the deposits. We show that low velocities correspond to the formation of monolayer and high velocities to multilayer. These new results are explained in terms of the local concentration of particles in the suspension near the contact line and the porosity of the pre-deposited structure. The effect of an applied electric field to the system is also reported.

1Partially supported by Departamento de Educación (Gobierno de Navarra)
2Supported by the Asociación de Amigos de la Universidad de Navarra
3See 2

8:12AM Y14.00002 Kinetics of formation and disintegration of ionic and non-ionic spherical micelles1, GUNJAN MOHAN, PPG Industries, DMITRY KOPELEVICH, University of Florida — Dynamics of self-assembly and structural transitions in amphiphilic systems play an important role in various industrial and biological processes. Main challenge in computational modeling of these dynamics is a complex interplay between various length- and time-scales. In this talk, we discuss development of a multi-scale model for formation and disintegration of non-ionic and ionic spherical micelles. This study is performed under the assumption that the dominant mechanism of micelle formation (disintegration) is a stepwise addition (removal) of individual surfactant monomers to (from) a surfactant aggregate. A series of molecular dynamics simulations is used to develop reduced stochastic models for these elementary processes. It is demonstrated that these processes involve complex interactions of the translational degree of freedom (i.e., distance between centers of mass of the aggregate and the monomer) with degrees of freedom corresponding to the monomer orientation and the micellar shape and microstructure.

1This research is supported by NSF

8:24AM Y14.00003 Using fluid flow to control the structure of soluble surfactants deposited through receding contact lines. BENJAMIN BEPPLER, KALYANI VARANASI, STEPHEN GAROFF, KRISTINA WOODS, Carnegie-Mellon University, GUENNADI EVMENENKO, Northwestern University — Moving contact lines are often used to deposit soluble organic molecules in applications such as spin coating and dip coating. In this study, we demonstrate that altering the flow field near such a contact line fundamentally changes the deposited surfactant structure. At slow contact line speeds, the substrate emerges dry. The rolling fluid motion near the contact line deposits a densely packed, tilted monolayer of surfactant along the emerging solid-vapor interface. Above a critical contact line speed, an evaporating thin film is entrained on the emerging substrate. Surfactant concentration constantly increases in this confined environment due to solvent evaporation. Monodisperse crystalline islands nucleate and grow on the substrate with sizes and shapes controlled by varying the deposition conditions. These results contrast with disordered deposits that result from evaporation at a pinned contact line. Our results suggest that dip-coating with control of dipping speed and evaporation rate produces unique assembled structures and may provide better control of deposition through moving contact lines.
8:36AM Y14.00004 Rapid Convective Deposition For Fabrication of Microlens Arrays
JAMES GILCHRIST, PISIST KUMNORKAEW, Department of Chemical Engineering, Lehigh University, NELSON TANSU, YIK-KHOON EE, Department of Electrical and Computer Engineering, Lehigh University — Micron-sized microspheres were deposited into thin films via rapid convective deposition, similar to the ‘coffee ring effect’ using a similar method to that studied by Prevo and Velev, Langmuir, 2003. By varying deposition rate and blade angle, the optimal operating ranges in which 2D close-packed arrays of microspheres existed were obtained. Previous models do not consider the effect of blade angle and blade surface energy on the deposition of the particles. Using a computer-aided scanning electron microscope, dynamic counts for particle engulfment and rejection by the dendrites during spin coating were revealed. The resulting microstructure controlled by varying the macro scale parameters and interaction between substrate and colloidal particles played an important role in formation of ordered crystalline arrays. These interactions were explored through a model comparing the residence time of a particle in the thin film and the characteristic time of capillary-driven crystallization to describe the morphology and microstructure of deposited particles. Fabricated microlens arrays assembled on LEDs using this process were demonstrated to enhance performance by 300%.

8:48AM Y14.00005 Permanent Flow-Induced Phase Transitions in Wormlike Surfactant Micelle Solutions
MUKUND VASUDEVAN, Cytec Industries Inc. Stamford, CT, ERIC BUSE, Washington University, Saint Louis, MO, AMY SHEN, University of Washington, Seattle, WA, BAMA KHOKAMI, University of Tennessee, Knoxville, TN, RAVINDKAR SURESHKUMAR, Washington University, Saint Louis, MO — It is well known that certain wormlike micelle solutions form flow-induced structures under shear flow. This structure transition is typically accompanied by an enhancement in the shear viscosity and the emergence of a new gel phase. However, such transitions are generally believed to be reversible, i.e., upon flow stoppage, the structure relaxes to equilibrium. In this work, we show that by subjecting translucent wormlike micelle solutions to high flow deformation over a rapid time scale, permanent flow-induced structures can be formed. We will discuss the phenomenology and plausible physical mechanisms underlying this discovery.

9:00AM Y14.00006 Understanding the structure of porous materials created by freeze casting
STEPHEN BARR, ERIK LULJET, University of Illinois at Urbana-Champaign — When a suspension of colloidal particles in water freezes, dendrites of ice with high aspect ratios are formed which can either engulf or reject the particles based on their size and the velocity of the advancing ice front. As the particles are pushed between the dendrites, concentrated regions of colloidal particles are formed. Recent experiments have shown that this can be exploited to create strong, lightweight, porous materials. We investigate this process using molecular dynamics simulations, focusing on the effect of the ice front velocity on the structure of the resulting material. We develop a simulation model which accounts for particle engulfment or rejection by the dendrites. We study both columnar and lamellar geometries. Our main finding is that variation of the front velocity not only affects the particle concentration in the interdendritic regions, but also the degree of order of the resulting solid.

9:12AM Y14.00007 End-Functionalized Triblock Copolymers as a Guide for Nanoparticle Ordering
RASTKO SKNEPNEK, JOSHUA ANDERSON, MONICA LAMM, JOERG SCHMALIAN, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Using molecular dynamics simulations we show that triblock copolymers, designed to have specific affinity for nanoparticles at the chain ends, can successfully mediate assembly of nanoparticle/copolymer composites. In this talk, we will present a detailed investigation of the phase diagram of these nanocomposites as a function of both nanoparticle size and concentration. We find a rich phase diagram with two striking features. The first is the existence of an unconventional square columnar phase of two interpenetrating line-lattices of micellar cylinders and aligned nanoparticles, and the second is a drastically enhanced stability of the gyroid phase. We interpret the origin of the square columnar phase by making an analogy to the packing of binary mixtures of disks. Based on the analysis of stretching of copolymers we argue that nanoparticles help stabilize gyroid order and drastically widen the region of its stability. Our study suggests that combining nanoparticles with functionalized block copolymers can provide a simple and efficient tool for assembling novel materials with nanometer scale resolution.

9:24AM Y14.00008 Unexpectedly wide distributions in the stochastic synthesis of functionalized nanoparticles
JACK WADDELL, DOUGLAS MULLEN, BRADFORD ORR, MARK BANASZAK HOLL, LEONARD SANDER, University of Michigan — Functionalized nanoparticles are promising devices with a variety of applications, such as the targeted delivery of chemotherapy drugs to cancer cells. Their properties depend on the specifics of the distribution of functional groups on the nanoparticle. Stochastic ligand conjugation is an efficient strategy for synthesizing large quantities of functionalized nanoparticles. We developed a kinetic model for the study of ligand distribution on a generation 5 poly(amideamine) dendrimer, as measured by HPLC and SPR. We found a cooperative effect in single species ligandation, leading to a broader-than-Poisson distribution of ligands on nanoparticles, and suggesting a high spatial correlation of functional groups.

9:36AM Y14.00009 Self assembly of silica nanoparticles in a surfactant mesophase
K. SHARMA, Ph.D. student, K. GURUSWAMY, Scientist, O. MONDAIN-MONVAL, Professor, I. LY — We examine the organization of silica particles in a hexagonal mesophase of a non-ionic surfactant, C_{12}E_8 in water. The mesophase has a characteristic length scale (cylinder-center-to-center distance, \(a\sim 5.7\) nm). We vary the size of the silica particles from \(\sim 2\) nm \((<a)\) to \(\sim 500\) nm \((>a)\), to examine the effect of particle size, and use a combination of SAXS, freeze fracture TEM and optical microscopy to characterize our materials. We show that particles \(<a\) behave like a solvent and template the mesophase. Particles with a size \(a\) are partitioned into a dispersed phase and into strand-like aggregates. Particles \(>a\) separate from the mesophase and form strand-like aggregates that organize into a network. The formation of this network is reversible and heating into the high temperature isotropic phase leads to dispersion of the particles. Unusually an increase in hexagonal-isotropic transition temperature is seen for the mesophase-particle composites. We show that the network forms by expulsion of the particles from growing hexagonal phase domains — as these domains grow, the particles are concentrated in the isotropic regions until they jam to form the network. We show that we are able to tune the mesh size of the particulate networks by changing the cooling rate.

Friday, March 20, 2009 8:00AM - 11:00AM — Session Y15 DFD: Liquid Crystals III

8:00AM Y15.00001 Magnetic-field induced isotropic to nematic liquid crystal phase transition
J.T. GLEESON, T.B. OSTAPENKO, Kent State University, D. B. WIANT, Wake Forest University, S.N. SPRUNT, A. JAKLI, Kent State University — We report on measurements of magnetic field induced nematic order in the bent-core liquid crystal 4-chlororesorcinol bis[4-(4-n-dodecylxyloxybenzoxyl) benzolate]. Using the 31 Tesla solenoid at the National High Magnetic Field Laboratory, we have observed, at temperatures less than one degree above the clearing point, a first-order transition to the nematic phase. The critical magnetic field at which this occurs increases with temperature. We discuss these results within the context of both Mater-Saupe and Landau-Ginzburg mean field models for the nematic-isotropic transition. The implications of this transition for the mesophase stability of the liquid crystal were also discussed. To our knowledge, this is the first observation of such a magnetic field-induced transition in a thermotropic liquid crystal; the reasons for which this behavior is now attainable are discussed.
This work was supported by the NSF (DMR-0606160) and Kent State University. Work performed at NHMFL supported by NSF cooperative agreement DMR-0084173, the State of Florida and the DOE.
8:12AM Y15.00002 High Magnetic Field-Induced Birefringence in Lyotropic Chromonic Liquid Crystals, T. OSTOPENKO, Kent State University, YU. NASTISHIN, Inst. for Phys. Opt., Lviv, Ukr., J.T. GLEESON, S.N. SPRUNT, O.D. LAURENTOVICH, Kent State University, P.J. COLLINGS, Swarthmore College — We studied the effect of magnetic-field induced birefringence of a 14% solution of disodium cromoglycate (DSCG) in water at temperatures above the nematic-isotropic coexistence region. According to Landau-deGennes mean field theory, we expect to find a linear relationship between the inverse of the induced birefringence, $\Delta n$, and the quantity (T-$T^*$), where $T^*$ is the stability limit of the isotropic phase. Using the 31 T resistive magnet at the National High Magnetic Field Laboratory, we observed that, as we increase the temperature above the coexistence region, we deviate from this linear dependence. Our data shows that $\Delta n$ goes to zero, whereas Landau-deGennes predicts that $\Delta n$ should decrease asymptotically. This may be due to the lack of isodense aggregate formation at a finite temperature above the coexistence region. Supported by NSF (DMR-0710544 and DMR-0606160). Work performed at NHMFL, supported by NSF cooperative agreements DMR-0084173, the State of Florida and the DOE.

8:24AM Y15.00003 ABSTRACT WITHDRAWN

8:36AM Y15.00004 Chromonic liquid crystalline properties of dyes, XUXIA YAO, JUNG PARK, School of Polymer, Textile, and Fiber Engineering, Georgia Institute of Technology, MOHAN SRINIVASARAO, School of Polymer, Textile, and Fiber Engineering, School of Chemistry and Biochemistry, Georgia Institute of Technology — As a new class of lyotropic liquid crystals, chromonic liquid crystals (CLCs) can self-assemble into an ordered complex fluid, potentially useful for organic solar cells. Different from common amphiphilic lyotropic mesophases, CLCs have no optimum aggregation size, which implies the order parameter increases with concentration. We used capillary flow and magnetic field to induce alignment in chromonic dyes and studied the aggregation behavior by Vis-spectroscopy, the phase behavior by POM and DSC, and the order distribution by Raman Scattering. We also investigated how the molecular structures influence the structures of mesogens and the morphology in the dried film which will further influence the charge mobility in the solar cells.

8:48AM Y15.00005 Liquid Crystalline Phase Transition of Colloidal Platelets with Identical Thickness1, DAZHI SUN, ZHENDONG CHENG, HUNG-JUE SUE, Texas A&M University, PROF. SUE’S TEAM, PROF. CHENG’S COLLABORATION — The disorder – order transition in discotic colloids has been an active research area since the observation of the nematic phase in clay suspensions by I. Langmuir in 1938. In the past decade, synthetic platelets have been used extensively to investigate the discotic liquid crystal phase transitions. Here, we report the phase behavior of a new model platelet system – alpha-zirconium phosphate (ZrP). After exfoliation, the monolayer ZrP platelets possess uniform thickness, but have a high polydispersity in diameter. We observed an isotropic - nematic transition in our system upon increasing the platelet volume fraction, followed by the formation of the discotic smectic phase, an elusive phase that has been rarely seen in discotic liquid crystals. The discotic smectic phase (domain) is characterized by X-ray diffraction, high-resolution transmission electron microscopy, and optical microscopy. The equation of state (EOS) of our system is also discussed.

1Special thanks are given to The Dow Chemical Company for their partial financial support. Acknowledgment is also made to the donors of the American Chemical Society ACS Petroleum Research Fund (RPF# 43053-G7).

9:00AM Y15.00006 Study of the Isotropic-Nematic and the Nematic-Smectic-A Phase Transitions in Carbon Nanotubes and Liquid Crystal Composites, KRISHNA SIGDEL, GERMANO IANNACCCHIONE, Worcester Polytechnic Institute — A high-resolution ac-thermal study of the isotropic to nematic (I-N) and the nematic to smectic-A (N-SmA) phase transitions of carbon nanotubes (CNTs) and liquid crystal octyl-cyanobiphenyl (8CB) composites (8CB+c-CNTs) as a function of CNTs concentration is reported. Scans were performed on heating and cooling for all samples (0.5-6 wt% of CNTs) over a wide temperature range well above and below the two transitions in pure 8CB. Both the I-N and the N-SmA transitions evolve in character and have their transition temperatures shift lower as the wt% of CNTs increases. For intermediate wt% values, new transitions features are observed, which suggest new phase ordering of the CNTs within the liquid crystal host.

9:12AM Y15.00007 Recovery and stabilization of a reversed phase sequence in a ternary liquid crystal mixture, RONALD PINDAK, Brookhaven National Lab, SHUN WANG, LIDONG PAN, Univ. of Minnesota, B.K. MCCOY, Azusa Pacific Univ., SUNTAO WANG, Brookhaven National Lab, H.T. NGUYEN, Univ. Bordeaux, CHENG-CHER HUANG, Univ. of Minnesota — The nOHFBBB1M7 (n = 10) compound, 100HF, shows a reversed SmC*$_{F12}$ - SmC* phase sequence, unique among all known antiferroelectric liquid crystals. This reversed phase sequence is stabilized upon doping with 90TBBB1M7(C9) or 110TBBB1M7(C11). In contrast, doping with homologous compounds (n = 9, 11, or 12) eliminates the SmC*$_{F12}$ phase. One 100HF/110HF mixture without the SmC*$_{F12}$ phase was selected for further studies. Adding C9 into this mixture revives the reversed phase sequence. Unexpectedly, even though 110HF destabilizes the SmC*$_{F12}$ phase in binary mixtures with 100HF, it significantly increases the SmC*$_{F12}$ temperature range in 100HF/110HF/C9 ternary mixtures. The extended temperature range is important for device applications.

9:24AM Y15.00008 Room-Temperature Liquid Crystal Blue Phases, STEFANIE TAUSHANOFF, Kent State University, KHOA VAN LE, Tokyo Institute of Technology, ROBERT TWIENG, ANITAL JAKLI, Kent State University — The “blue phases” of a highly chiral liquid crystal are defect-studded structures of double-twist cylinders that are laced together. The three phases, BP1*, BP2* and BP3* differ in the packing of the double-twist cylinders. Until recently, blue phases were of limited practical use because they appeared for only a very narrow temperature range. Mixtures that show BP1* and BP2* phases for wide temperature ranges at or around room temperature are now available [1]. Relatively wide temperature BP3* (the blue fog) phase so far is available only at very high temperatures [2]. Here we present mixtures with room-temperature wide range BP2* phase and compare the ability of chiral dopants to form the different blue phases in a base nematic mixture. PDLC films cast with blue-phase material are also examined.


9:36AM Y15.00009 Hybrid shells of nematic liquid crystal, ALBERTO FERNANDEZ-NIEVES, TERESA LOPEZ-LEON, Georgia Tech — We investigate the consequences of changing the boundary conditions for the nematic director at the outer surface of a spherical shell from planar to homeotropic. We find there are different routes to the final equilibrium configuration, depending on the initial shell structure. For bipolar shells, which are shells having two pairs of $s=\pm 1/2$ boojums on either surface, a disclination ring forms, shrinks and disappears in a process that is highly reminiscent of that seen in bipolar drops. By contrast, shells with four $s=\pm 1/2$ defects develop open disclination lines in the inner surface; these lines form between the original $s=\pm 1/2$ defects and force their approach and coalescence. These results highlight the fascinating range of behaviors that are driven by the interplay between topological constraints and the nematic order of liquid crystals.
to better account for the highly aligned segments. This method allows us to probe the chain segment alignment with increasing strain in both unimodal and
S caused by excluded volume interactions between neighboring segments. We synthesized deuterated PDMS chains of about 5000 g/mol and 80,000 g/mol
orientation in elastomers is revealed by solid state deuterium NMR spectra: earlier work has focused on the frequency split between the peaks of the spectra
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cycled into magnetic field during SmA–I transition to get an aligned matrix of nanocolloids. Heating scans were performed at various heating rates from 20
by solvent dispersion method (SDM) where different densities of aerosil nanoparticles were added into octyl-cyanobiphenyl liquid crystal. Then samples were
(interesting thermal behavior of an aligned aerosil nano-colloidal system in the aligned matrix of octyl-cyanobiphenyl liquid crystal. This system was prepared,
DiPTI SHARMA, UML — This study investigates an in-
10:12AM Y15.00012 Second Harmonic Generation in a Bent-core Nematic Liquid Crystal.1
, SEUNG HO HONG, ANTAL JAKLI, JAMES GLEESON, SAMUEL SPRUNT, BRETTT ELLMAN, Kent State University — We studied second harmonic
generation (SHG) as a function of optical polarization in a magnetically-aligned bent-core nematic liquid crystal (BCN). At the isotropic to nematic transition
we detect the onset of a weak SH signal, which stays approximately constant through the nematic phase. Our results for polarization selectivity and for cells of
different thickness indicate that the signal from the BCN cannot be explained by quadrupoles, defects in director orientation, fluctuations or cell-surface
polarization. We discuss models for a noncentrosymmetric component of the BCN structure that can explain our data.

1Work supported by NSF DMR0606160.

10:24AM Y15.00013 Viscoelastic parameters and flexoelectric effect in a bent-core nematic liquid crystal studied by dynamic light scattering
. MADHABI MAJUMDAR, K. NEUPANE, JAMES T. GLEESON, ANTAL JAKLI, SAMUEL SPRUNT, Kent State University — Recent measurements of the flexure-induced
electric polarization in certain bent-core nematics (BCNs) have demonstrated a giant flexoelectric effect [1]. We present a study of nematic elasticities and viscosities in one of these compounds, together with an attempt to characterize the flexoelectricity by its effect on director fluctuations. Our results combined with a reanalysis of earlier data indicate that the flexoelectricity is a phenomenon distinct from the ordinary director modes; additionally we observe unusual, very slow fluctuations in polarized scattering which suggest the BCN has a heterogeneous, “glassy” character. Dilution in a miscible calamitic indicates a dramatic development of the slow dynamics between 30 wt % and 60 wt % BCN. We suggest a model to account for both our present results and the giant flexoelectricity discovered in [1]. Reference: [1] J. Harden et al., Phys. Rev. Lett., 97, 157802 (2006). Acknowledgement: NSF DMR-0606160.

10:36AM Y15.00014 Large Flow-Birefringence of Nematogenic Bent-Core Liquid Crystals
. CHRISTOPHER BAILEY, Kent State University, KATALIN FODOR-CSORBA, Research Institute for solid state physics and optics, Budapest, Hungary,
RAFAEL VERDUZCO, Oak Ridge National Laboratory, JAMES GLEESON, SAMUEL SPRUNT, ANTAL JAKLI, Kent State University — We have found that bent-core liquid crystalline materials show exceptionally large flow birefringence in their isotropic liquid phase. The flow birefringence is over two orders of magnitude larger than usual for low molecular weight liquid crystals. Comparing the flow birefringence per unit viscosity, the observed values are an order of magnitude larger than low molecular weight and side-chain polymeric calamatic liquid crystals. This large flow birefringence is attributed to the nanostructure of these materials that contain temporary smectic clusters of a few smectic layers, which exist even in their isotropic phase. These smectic clusters appear to shear align resulting in the observed flow birefringence behavior.

10:48AM Y15.00015 Activated Kinetics of Nematic and Smectic Phase Transitions in an
Aligned Matrix of Nano-colloidal Liquid Crystalline Gel
. DIPTI SHARMA, UML — This study investigates an interesting thermal behavior of an aligned aerosil nano-colloidal system in the aligned matrix of octyl-cyanobiphenyl liquid crystal. This system was prepared by solvent dispersion method (SDM) where different densities of aerosil nanoparticles were added into octyl-cyanobiphenyl liquid crystal. Then samples were cycled into magnetic field during SmA–I transition to get an aligned matrix of nanocolloids. Heating scans were performed at various heating rates from 20 to 1 K min−1 using DSC. Aligned samples follow Arrhenius behavior and showed a decrease in transitions temperature for SmA–N and N–I transitions when compared with the unaligned samples. The activation energy of the aligned system increases and its respective enthalpy decreases for the lowest density of aerosils 0.05 g cm−3, then for the further increase of aerosil density, the activation energy decreases and its respective enthalpy increases. The second order transition SmA–N shows a higher activated kinetics than the weak first order N–I transition. This can be explained in terms of molecular interaction between aerosil nanoparticles and aligned liquid crystal molecules, and developed strain in the matrix of the aligned system.

Friday, March 20, 2009 8:00AM - 11:00AM –
Session Y16 DPOLY: Elastomers and Gels II 317

8:00AM Y16.00001 Deuterium NMR studies of segment orientation in PDMS unimodal and
bimodal endlinked networks.1
, CLAUDE COHEN, GEOFFREY GENESKY, T. MICHAEL DUNCAN, Cornell University — Polymer segment orientation in elastomers is revealed by solid state deuterium NMR spectra: earlier work has focused on the frequency shift of the spectra from stretched elastomers rather than the details of the lineshape. The split has classically been interpreted as a measure of polymer segment order parameter S caused by excluded volume interactions between neighboring segments. We synthesized deuterated PDMS chains of about 5000 g/mol and 80,000 g/mol to probe the segmental orientation of each component separately in bimodal networks. Even in the unstretched state, the spectra for the labeled short chain networks show an evolving lineshape with varying short chain content. We compute the average absolute value of the frequency shift of the entire spectrum to better account for the highly aligned segments. This method allows us to probe the chain segment alignment with increasing strain in both unimodal and bimodal networks and confirms Monte Carlo simulation results.

1NSF Polymers Program DMR-0705665
8:12AM Y16.00002 Volume-phase Transitions and Confined Water in Surface-tethered Poly(N-isopropylacrylamide) Networks, AJAY VIDYASAGAR, RYAN TOOMEY, University of South Florida — We present a simple approach for studying volume-phase transitions in thin, mechanically anchored responsive polymer networks. The approach is based on the photo-cross-linking of copolymers synthesized from N-isopropylacrylamide NIPAAm) and methacryloyloxybenzophenone (MaBP). We monitored the swelling of poly(NIPAAm-co-MaBP) networks in contact with aqueous solution at a function of cross-link density with both neutron reflection and ATR-FTIR. Neutron reflection reveals that the volume-phase transition of tethered poly(NIPAAm) networks coincides with the miscibility gap of linear poly(NIPAAm) solutions. Whether or not the poly(NIPAAm) network undergoes a continuous or discontinuous collapse depends on its degree of cross-linking. At cross-link densities above 5 mole%, the network remains in the single-phase region of the linear solution phase diagram and shows only a continuous transition between the swollen and collapsed states. Moreover, in the collapsed state, 30-35% by volume of water remains in the network, which is independent of cross-link density. The relative position of the FTIR absorption peaks during the collapse follows very closely the amount of water in the layer and can be related to the local dielectric environment within the network.

8:24AM Y16.00003 Strain induced alignment of particles in an elastomer host, BEN SPOTT, JEREMY NEAL, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — The properties of composite materials consisting of anisometric nanoparticles depend on the orientation of the nanoparticles. It is interesting to ask how mechanical strain of the composite affects their orientation. We have carried out experiments stretching both two- and three-dimensional rubber samples containing rigid rod-like particles and measured their orientational order parameter as a function strain. We discuss these results, and make connections with theoretical models.

3 This work was supported by the AFOSR under MURI grant FA9550-06-1-0337.

8:36AM Y16.00004 Dynamics of uniaxially oriented elastomers using dielectric spectroscopy, HYUNGKI LEE, DANIEL FRAGIADAKIS, Penn State University, DARREN MARTIN, University of Queensland, JAMES RUNT, Penn State University — We summarize our initial dielectric spectroscopy investigation of the dynamics of oriented segmented polyurethanes and crosslinked polyisoprene elastomers. A specially designed uniaxial stretching rig is used to control the draw ratio, and the electric field is applied normal to the draw direction. For the segmented PU s, we observe a dramatic reduction in relaxation strength of the soft phase segmental process with increasing extension ratio, accompanied by a modest decrease in relaxation frequency. Crosslinking of the polyisoprene was accomplished with dicumyl peroxide and the dynamics of uncrosslinked and crosslinked versions are investigated in the undrawn state and at different extension ratios. Complimentary analysis of the crosslinked PI is conducted with wide angle X-ray diffraction to examine possible strain-induced crystallization, DSC, and swelling experiments. Quantitative analysis of relaxation strengths and shapes as a function of draw ratio will be discussed.

3 Supported by the NSF Polymers Program, DMR-0605627.

8:48AM Y16.00005 Shape-Memory Polymers Based on Fatty Acid-Filled Elastomeric Ionomers, ELISE IZZO, ROBERT WEISS, University of Connecticut — Shape memory polymers (SMPs) have applications as medical devices, actuators, sensors, artificial muscles, switches, smart textiles, and self-deployable structures. All previous design of SMPs has involved synthesizing new polymers or modifying existing polymers. This paper describes a new type of SMP based on blends of an elastomeric ionomer and low molar mass fatty acids or their salts (FAS). Shape memory elastomers were prepared from mixtures of a sulfonated EPDM ionomer and various amounts of a FAS (e.g., zinc stearate, zinc oleate, and various aliphatic acids). Nanophase separation of the metal sulfonate groups provided the “permanent” crosslinks, while sub-microscopic crystals of the low molecular weight FAS provided a physical crosslink needed for the temporary shape. The material was deformed above the melting point of the FAS and the new shape was fixed by cooling the material while under stress to below the melting point of the FAS. Polar interactions between the ionomer and the FAS stabilized the dispersion of the FAS in the polymer and provided the continuity between the phases that allowed the crystals of the FAS to provide a second network of physical crosslinks. The temporary shape was erased and the material returned to the primary shape by heating above the melting point of the FAS.

9:00AM Y16.00006 Dynamics of Segmented Polyurethane Elastomers Using Dielectric Spectroscopy, JAMES RUNT, The Pennsylvania State University, DANIEL FRAGIADAKIS, ALICIA CASTAGNA, TAEYI CHOI — This investigation focuses on the molecular dynamics of segmented polyurethane copolymers with different hard segment contents (30 to 52 wt percent) and soft segment chemistries. Methylene bis(p-phenyl isocyanate) and 1,4-butanediol constitute the hard segments in all materials under investigation, while soft segments include poly(tetramethylene oxide) and a 80-20 mixture of poly(dimethylsiloxane) and poly(hexamethylene oxide). The dynamics of these materials were explored over a wide temperature and frequency range using dielectric spectroscopy. In addition to investigating the details of segmental and local processes, three dielectric relaxations above Tg were observed for the first time in segmented polyurethanes, and their origin discussed in the presentation. For example, the highest temperature process is assigned to Maxwell-Wagner-Sillars interfacial polarization. The strength of the MWS process is a sensitive indicator of the change in microphase-separated character. It disappears at a temperature similar to that at which the small-angle X-ray scattering maximum disappears, indicating the transformation to the single phase state.

9:12AM Y16.00007 Polydomain to monodomain transition in nematic liquid crystal elastomers, BADEL MBANGA, FANGFU YE, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute / Kent State University — Liquid crystal elastomers are crosslinked polymer networks covalently bonded with liquid crystal mesogens. In the nematic phase, due to strong coupling between mechanical strain and orientational order, these materials display strain-induced instabilities associated with formation and evolution of orientational domains. Deformation of an initially polydomain nematic elastomer film induces a transition to the monodomain configuration. We model this phenomenon using a recently developed finite element elastodynamics simulation method. We study the rate-dependent material response upon uniaxial extension and resolve the textures that form along with the associated stress-strain behavior. Our simulations yield qualitative agreement with experimental observations. This model allows us to explore the fundamental physics governing dynamic mechanical response of nematic elastomers and also provides a potentially useful computational tool for engineering device applications.

3 Supported by U.S. National Science Foundation DMR-0605889.
**9:24AM Y16.00008 Liquid crystal elastomers: Bent core flexoelectricity**¹, MARTIN CHAMBERS, Liquid Crystal Institute and Physics Department, Kent State University, Kent OH44240, USA, RAFAEL VERDUZZO, Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge TN37831, USA, SAMUEL SPRUNT, JAMES T. GLEESON, Physics Department, Kent State University, ANTAL JAKLI, Liquid Crystal Institute, Kent State University — We report on the swelling of calamatic liquid crystal elastomers (LCE) with bent-core mesogens (BCM); this swelling took place at a temperature where both materials were in their isotropic phase. The BCM used varied in the degree of saturation of their hydrocarbon tails, which affects both viscosity and phase behaviour. We determined both swelling magnitude and dynamics. The host LCE systems homogeneously imbibe BCM up to 30-40 mol. Based on differential scanning calorimetry, shape change anisotropy, and optical birefringence measurements, the swollen elastomers are all found to exhibit nematic phases, with some possessing a lower temperature smectic phase. Bent-core liquid crystal elastomers and swollen calamatic LCE in BCM were investigated for the flexoelectric properties by inducing a mechanical deformation. The value of the bend flexoelectric constant, e_{ij} of the swollen BCM containing LCE systems is comparable to that of the neat bent-core liquid crystal.

¹This work was supported by the ONR (N00014-07-1-440).

**9:36AM Y16.00009 Photoinduced distortions of polydomain liquid crystal elastomer samples**¹, WILDER IGLESIAS, PETER PALFFY-MUHORAY, Liquid Crystal Institute, Kent State University — We have studied the effects of illumination of a dye doped polydomain nematic elastomer. The sample was on a glass substrate, and its free surface was illuminated by polarized light from an Ar+ laser. The shape of the reflected light in the far field was studied to probe photoinduced deformations. Above a threshold intensity, a target pattern appeared in the far field, indicating sample deformation. We discuss the experimental observations, and relate these to the processes such as photoinduced surface relief. Experimental results are compared with the predictions of simple theory.

¹This work was supported by the NSF under grant DMR 0606357.

**9:48AM Y16.00010 Dynamic Aspect of Electro-Opto-Mechanical Effects in Swollen Nematic Elastomers**, KENJI URAYAMA, ATSUSHI FUKUNAGA, TOSHIKAZU TAKIGAWA, Dept. Mater. Chem., Kyoto Univ., ANTONIO DESIMONE, SISSA, LUCIANO TERESI, SMFM, Univ. Roma III, KYOTO UNIV. TEAM, SISSA COLLABORATION, UNIVERSI ROMA III COLLABORATION — The nematic elastomers swollen by low molecular mass liquid crystals exhibit a macroscopic deformation with a significant change in birefringence in fast response to electric fields. We experimentally characterize the dynamics of this "electro-opto-mechanical effect." The optical and mechanical rise times (in response to field-on) decrease in nearly proportion to the square of field strength, while the corresponding decay times (in response to field-off) are almost independent of field strength. The optical rise and decay times are about one order magnitude smaller than the mechanical ones. We also propose a minimal model to describe the main features of both static and dynamic characteristics of this phenomenon observed experimentally. 1) Urayama, K., Honda, S., Takigawa, T., Macromolecules, 2006, 39, 1943. 2) Fukunaga, A., Urayama, K., Takigawa, T., DeSimone, A., Teresi, L., Macromolecules, in press.

**10:00AM Y16.00011 Analysis of Diffusion through Dynamic Network Polymers using Multi-photon Fluorescence Recovery after Photobleaching**, JIAHUI LI, Department of Chemical Engineering, University of Rochester, KELLEY SULLIVAN, EDWARD BROWN, Department of Biomedical Engineering, University of Rochester, MITCHELL ANTHAMATTEN, Department of Chemical Engineering, University of Rochester — Multi-Photon Fluorescence Recovery after Photobleaching (FRAP) techniques are utilized to study small molecule transport through polymer networks containing multiple hydrogen-bonding functional groups. Experiments involve uniformly dispersing small dye molecules (fluorophores) into functionalized polymers and networks. Polymer samples are then locally bleached, and the recovery of fluorescence is studied using 2-photon fluorescence microscopy. By curve-fitting fluorescence recovery curves to a model, diffusion coefficients are obtained. We have investigated series of polymer networks containing H-bonding interactions with different compositions at different temperatures. The diffusion coefficient through these polymer networks shows an expected Arrhenius-like temperature dependence. The influence of hydrogen bonding and network architecture on transport activation energies will be discussed.

**10:12AM Y16.00012 Gelling Mechanism of Aluminum Di-Soaps in Oils**, XIAORONG WANG, Bridgestone Americas, Center for Research and Technology, 1200 Firestone Parkway, Akron, OH 44317, MINDAUGAS RACKAITIS — This work demonstrates that aluminum di-soaps form nano-sized spherical micelles in the oils and that the aggregation of these micelles forms a network that gives rise to a gel formation – thereby refuting a long-held belief that the gel formation was the result of linear polymeric chains of aluminum association. The discovery of such aluminum nano-particles could expand application of these materials to new technologies because these materials are chemically inert, odorless and nontoxic, and have been widely used in greases, paints, gels, cosmetics, drugs and foods.

**10:24AM Y16.00013 Surface Plasmon Resonance Effects in Responsive Polyelectrolyte/Gold Nanoparticles Hydrogel Thin Films**¹, IHOR TOKAREV, IRYNA TOKAREVA, VENKATESHWARLU GOPISHETTY, SERGIY MINKO, Clarkson University — In this study, we explored localized surface plasmon resonance excited in gold nanoparticles coupled with continuous and macroporous stimuli-responsive hydrogel thin films. The 100-nm-thick porous hydrogel film with vertically aligned cylindrical pores decorated with spherical Au nanoparticles (synthesized in the hydrogel) and placed on Au islands (prepared on a glass substrate) enabled the highly-sensitive optical detection of changes in the swelling degree of hydrogel induced by an external stimulus (pH). The strong optical response of our sensing platform is attributed to the electromagnetic coupling between the nanoparticles and islands that is highly sensitive to the inter-particle spacing. The transformation of a chemical signal into the optical effect can be used for analytical applications.

¹This work was supported by NSF DMR-0706209 and U.S. ARO W911NF-05-1-0339 grants.

**10:36AM Y16.00014 Gelation, Dynamics and Mechanics of Associating Polymers: Exploring Parameter Space**, ROBERT S. HOY, GLENN H. FREDRICKSON, Materials Research Laboratory, University of California, Santa Barbara — We present simulation studies of associating polymer melts, where a fraction of the monomers are “sticky.” A coarse grained hybrid MD/MC model is used to accurately model polymer dynamics and qualitatively capture chemical kinetics. The effects of varying sticky bond strength, sticky monomer concentration and placement along chains, chain length N, temperature T, and chemical kinetics are examined. All have independent and interesting effects on the dynamics and mechanics. We focus on the “reversible” gel regime where almost all chains are instantaneously connected to the network, yet chains are delocalized and the system displays complex time and strain-dependent properties.
We present a theoretical analysis of a novel cavity electromechanical (or optomechanical) system where a mechanical resonator directly modulates the damping in obtaining information on the raw key in quantum key distribution. This construction essentially proves the intuition that separate measurements on the subsystems are sufficient to extract the maximal information about the separately prepared, we construct separate measurements on the subsystems from any given joint measurement such that the former always give at least as large information as the latter. This construction offers new insights into the understanding of measurements on this type of composite systems. Moreover, this effective model is derived, showing how coherent transfer between both two level systems can be achieved, and the possible advantages of the system as the standard quantum limit. Finally, we will outline several exciting applications of the novel magnetic sensors in areas ranging from bio- and materials science to electronic spin bath. As an outlook, we will discuss how engineering, controlling or harnessing the environment can lead to better sensitivity, even beyond the standard quantum limit. We also show that this system can be used to perform quantum-limited position measurements. The system described here could be implemented directly using setups similar to those used in recent experiments in cavity electromechanics.

10:48AM Y16.00015 Step Cycle Deformation Processing of Elastomers and Gels Based on Semicrystalline Polyolefin-based Block Copolymers, FANNY DEPLACE, ZHICANG WANG, NATHANIEL A. LYND, ATSUSHI HOTTITRA, GLENN H. FREDRICKSON, EDWARD J. KRAMER, UC BERKELEY - SCIENCE, Cornell University, HISAHI OHTAKI, K. HIROKANE, F. YAMADA, YONG-WOOL SHIN, FUMIHIKO SHIMIZU, Mitsubishi Chemical Group, Science and Technology Research Center — Recent catalysts have enabled the synthesis of block copolymers with semicrystalline syndiotactic and isotactic polypropylene endblocks and amorphous ethylene-propylene midblocks. In these copolymers, the crystals play the role of physical crosslinks which can deform plastically under stretching. Neat elastomers, gels in mineral oil and gels from which mineral oil has been extracted have been subjected to step cycle tensile tests. The incremental plastic deformation of the crystals has dramatic effects on the true stress versus extension ratio curves. Moreover, small and wide angle X-ray scattering experiments during step cyclic tests revealed the evolution of the microstructure of the crystalline blocks: crystal fibrils and crystals in the fibrils are oriented parallel to the tensile direction at large strains and once the stress has decreased to zero, the fibrils return to being randomly oriented again.

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8:00AM Y17.00001 High-sensitivity diamond magnetometer with nanoscale resolution, PAOLA CAPPELLARO, ITAMP - Harvard Smithsonian CfA and Physics Department — We will discuss our recent work on using isolated electronic spins in the solid-state as sensitive magnetic sensors [1,2]. This novel approach to magnetometry is enabled by the good coherence properties of electronic qubits, such as the spins associated with Nitrogen-Vacancy (NV) centers in diamond, as well as by advanced techniques for their coherent control. The key feature of this solid-state magnetometer is the possibility to confine the sensing spins into a crystal of nanometer size that can be brought extremely close to the magnetic field source, thus achieving high spatial resolution. Our first experiments demonstrate that the resulting magnetic sensor provides an unprecedented combination of ultra-high sensitivity and spatial resolution. The ultimate sensitivity limit is set by the interaction of the spin sensor with its environment and in particular the nuclear and electronic spin bath. As an outlook, we will discuss how engineering, controlling or harnessing the environment can lead to better sensitivity, even beyond the standard quantum limit. Finally, we will outline several exciting applications of the novel magnetic sensors in areas ranging from bio- and materials science to fundamental physics and single electronic and nuclear spin detection.


8:36AM Y17.00002 Coupling Nitrogen Vacancy Centers in a Diamond Nanopillar to a Silica Microsphere, KHODADAD DINYARI, MATS LARSSON, HAILIN WANG, Department of Physics, Oregon Center for Optics, University of Oregon, Eugene, Oregon 97403 — Nitrogen vacancy (NV) centers in a diamond nanopillar have been coupled to the whispering gallery modes (WGMs) of a silica microsphere. The NV centers were coupled to the WGMs by positioning a nanopillar near the equator of the microsphere with nanometer precision. For cavity QED studies, WGMs with ℓ = m are of interest due to their small mode volumes. It was observed that when a 200 nm diameter nanopillar was optimally coupled to this particular mode in a 50 μm diameter microsphere, the quality factor (Q) was only reduced to 2x10^9 from an initial Q of 6x10^10. The nanopillars were fabricated from a bulk single crystal diamond by means of reactive ion etching, resulting in nanopillars with diameters as small as 200 nm with a height of approximately 1 μm. We estimate that a 140 nm pillar would allow a cavity linewidth of order 20 MHz, comparable to the zero phonon linewidth of a NV center. Producing a nanopillar with a 140 nm diameter is well within our fabrication technique making this composite system a suitable candidate for strong-coupling cavity QED. This nanopillar-microsphere system circumvents the poor controllability of nanocrystal based microresonator systems and utilizes the exceptional properties of both NV centers in bulk crystals and the ultra-high Q of silica microspheres.

8:48AM Y17.00003 An Ensemble of NV-centers in Diamond Coupled to a Flux Qubit, DAVID MARCOS, Consejo Superior de Investigaciones Científicas, MARTIJN WUBS, Niels Bohr Institute, R. AGUADO, Consejo Superior de Investigaciones Científicas, M.D. LUKN, ANDERS SORENSEN, Niels Bohr Institute — In the last years, the interface between quantum optics and solid state physics has been explored, and various models for hybrid qubits have been proposed. We consider a superconducting flux qubit coupled to an ensemble of NV-centers in diamond. An effective model is derived, showing how coherent transfer between both two level systems can be achieved, and the possible advantages of the system as the building block of a quantum computer.

9:00AM Y17.00004 Getting Information on Independently Prepared Quantum States — When are Individual Measurements as Powerful as Joint Measurements?, CHI-HANG FRED FUNG, H. F. CHAU, University of Hong Kong — Given a composite quantum system in which the states of the subsystems are independently (but not necessarily identically) prepared, we construct separate measurements on the subsystems from any given joint measurement such that the former always give at least as large information as the latter. This construction offers new insights into the understanding of measurements on this type of composite systems. Moreover, this construction essentially proves the intuition that separate measurements on the subsystems are sufficient to extract the maximal information about the separately prepared subsystems, thus making a joint measurement unnecessary. Furthermore, our result implies that individual attacks are as powerful as collective attacks in obtaining information on the raw key in quantum key distribution.

1This work is supported by the RGC grant No. HKU 701007P of the HKSAR Government and NSERC of Canada.

9:12AM Y17.00005 Quantum noise interference as a route to ground state cooling in cavity electromechanics, AASHISH CLERK, FLORIAN ELSTE, Dept. of Physics, McGill University, STEVE GIVIN, Dept. of Physics, Yale University — We present a theoretical analysis of a novel cavity electromechanical (or optomechanical) system where a mechanical resonator directly modulates the damping rate \( \kappa \) of a driven microwave (or optical) cavity. We show that due to a destructive interference of quantum noise, the driven cavity can effectively act like a zero-temperature bath irrespective of the ratio \( \kappa / \omega_m \), where \( \omega_m \) is the mechanical frequency. This scheme thus allows one to cool the mechanical resonator to its ground state without requiring the cavity to be in the so-called good cavity limit \( \kappa \ll \omega_m \). This behavior is in sharp contrast to the more common setup with a parametric coupling (where the mechanics modulates the frequency of the cavity): there, ground state cooling is only possible in the good cavity limit [1,2]. We also show that this system can be used to perform quantum-limited position measurements. The system described here could be implemented directly using setups similar to those used in recent experiments in cavity electromechanics [3].

9:24AM Y17.00006 Force sensitivity of a nanomechanical oscillator in a microwave cavity. JENNIFER HARLOW, JOHN TEUFEL, TOBIAS DONNER, KONRAD LEHNERT, JILA, University of Colorado and NIST — We describe our efforts to realize ultrasensitive force detection based on sensing the motion of nanomechanical oscillators embedded in superconducting resonant microwave cavities. Such a force sensor requires a readout mechanism quiet enough that the sensitivity is limited by thermal noise of the oscillator, as we recently demonstrated [1]. Force sensitivity is optimized by low mass, high-Q mechanical resonators with MHz resonance frequencies. We report measurements with sub-nN/√Hz force sensitivity and discuss prospects for further progress. [1] C. A. Regal, J. D. Teufel, and K. W. Lehnert, Nature Physics 4, 555 (2008).

9:36AM Y17.00007 Resolved-Sideband Cooling of Nanomechanical Motion within a Microwave Cavity. JOHN TEUFEL, JENNIFER HARLOW, TOBIAS DONNER, MICHAEL DEMORET, KONRAD LEHNERT, JILA, University of Colorado and NIST — We present recent experiments in which we couple the motion of a high-Q nanomechanical oscillator to the microwave fields in a superconducting resonant circuit [1]. This microwave optomechanical system is operated in the resolved-sideband regime in which the mechanical resonance frequency exceeds the cavity bandwidth. In this regime, the dynamic backaction of the microwave radiation further cools the mechanical motion from dilution refrigerator temperatures to even lower thermal occupancy. Recent improvements increase both the optomechanical coupling strength and the power handling capability of the cavity. We report progress toward cooling to the mechanical ground state with this system. [1] J. D. Teufel, J. W. Harlow, C. A. Regal and K. W. Lehnert, Phys. Rev. Lett., 101, 197203 (2008).

9:48AM Y17.00008 Photon-Mediated Magnetic Cooling of a Micromechanical Oscillator. JOONHO JANG, RAFFI BUDAKIAN, Physics Department, University of Illinois at Urbana-Champaign — In recent years, a number of techniques have been developed to cool a mode of a micromechanical oscillator to the ground state. In this talk, I will present a new scheme for cooling a micromechanical oscillator involving the interaction of a micron-size superconductor, attached to the cantilever, with an external magnetic field. When the cantilever is placed inside an optical cavity, the absorption of photons by the superconductor gives rise to a retarded force that modifies the damping of the oscillator. Initial measurements using NbSe₂ show approximately a factor of 25 reduction in the mode temperature from 5 K to 200 mK. By optimizing the cavity finesse, the magnetic field configuration, and the superconductor quasiparticle lifetime, a further reduction of 10⁴ in the cantilever mode temperature could be realized.

10:00AM Y17.00009 Parametric Amplification and Detection of Nanomechanical Motion. JARED HERTZBERG, Department of Physics, University of Maryland, TRISTAN ROCHELEAU, TCHEFOR NDUKUM, KEITH SCHWAB, Department of Physics, Cornell University — We have performed experiments with a 5.57 MHz nanomechanical resonator (NR) capacitively coupled to a 5 GHz superconducting microwave resonator and cooled to a temperature of 142mK. When driving with two microwave tones, a configuration appropriate for back-action evading measurements of a single motional quadrature, we find that a parametric instability appears at high drive powers. Due to the interference of the microwave tones, the capacitive frequency shift of the NR is periodically modulated at twice the mechanical frequency, resulting in a degenerate parametric amplification of the mechanical motion. In this regime, we demonstrate mechanical gains of up to 11.6dB and parametrically reduced linewidths of 2.1 Hz, resulting in a position resolution near the standard quantum limit. Although this effect is expected to limit the back-action evasion dynamics, it is useful for mechanical preamplification and noise squeezing, subjects of future work.

10:12AM Y17.00010 Back action evading quantum limited measurements of a nanomechanical resonator. TCHEFOR NDUKUM, TRISTAN ROCHELEAU, Department of Physics, Cornell University, JARED HERTZBERG, Department of Physics, University of Maryland, KEITH SCHWAB, Department of Physics, Cornell University — By driving a 5GHz superconducting, co-planar waveguide (CPW) resonator coupled to a radio-frequency nanomechanical resonator with both red- and blue-detuned, phase coherent microwave signals, we demonstrate amplifier noise back action evading (BAE) detection of one quadrature of nanomechanical motion. With this method we show precise measurements of a single motional quadrature with additive measurement noise of 4 times the zero point amplitude, and a reduction in sensitivity to injected measurement noise of a factor of 43 in comparison to a single tone, non-BAE measurement. We have also found a parametric instability which limits the coupling strength possible in our device, which will be described elsewhere. With straightforward improvements to the microwave resonator, we expect to be able to demonstrate sensitivity to one quadrature with additive measurement noise below the zero-point level, a necessary ingredient to produce and measure squeezed states of motion.

10:24AM Y17.00011 Sideband Resolved Cooling of a Nanomechanical Resonator Parametrically Coupled to a Microwave Resonator. TRISTAN ROCHELEAU, TCHEFOR NDUKUM, JARED HERTZBERG, KEITH SCHWAB, Department of Physics, Cornell University — We have fabricated a nanostructure formed by a radio-frequency nanomechanical (NEMS) resonator capacitively coupled to an aluminum 5 GHz superconducting, co-planar waveguide (CPW) resonator with 50 Ω characteristic impedance. By driving this coupled system at a frequency ω_pump = ω_CPW - ω_NEMS, we demonstrate back action cooling effects of a single NEMS mode achieving cooling from temperatures of 100mK to <10mK, with the lowest occupation factor of N<30. We have recently demonstrated a Nb, 130 Ω 5 GHz, Q=15,000 microwave resonator which we expect to be capable of cooling the NEMS close to ground state.

10:36AM Y17.00012 Ground state cooling of nanomechanical resonator via linear coupling in a superconducting circuit¹. LIN TIAN, School of Natural Sciences, University of California, Merced, CA 95344 — In recent experiments, it has been demonstrated that radiation pressure-like coupling between a nanomechanical resonator and a superconducting resonator can be explored for the cooling of the nanomechanical mode. In this work, we present a ground state cooling scheme for a nanomechanical resonator linearly coupled with a superconducting LC oscillator. The linear coupling, when periodically modulated at red detuning, up-converts the low-frequency nanomechanical mode to the high-frequency LC oscillator mode and generates backaction force that can cool the nanomechanical mode to its ground state in the resolved-sideband regime. Compared with schemes using radiation pressure-like coupling, the LC oscillator mode doesn’t need to be driven to high photon occupation number in our scheme. We calculate the cooling rate and the stationary occupation number of the nanomechanical mode and show that ground state can be reached with practical device parameters. A detailed study of our model shows that the quantum backaction noise that limits the cooling process is due to the counter rotating terms in the linear coupling. The scheme can be compared with laser cooling for the atomic systems as well.

¹The work is in part supported by the Karel Urbanek Fellowship at Stanford University.

10:48AM Y17.00013 Quantum Measurements of Coupled Systems. L. FEDICHKIN, M. SHAPIRO, M. I. DYKMAN, Michigan State University — Quantum measurements are often performed on coupled systems. Such measurements are of interest for various proposed applications of a quantum computer where the qubit-qubit coupling may not be completely turned off. Because of the coupling, the stationary state wave functions are not fully localized on individual qubits even where the energies of neighboring qubits are tuned away from each other. As a result, an instantaneous projective single-qubit measurement gives the state population with an error. We show that the error may be significantly reduced. This is accomplished by tuning the detector close to resonance with the measured qubit. The qubit- detector coupling should be small compared to the decay width γ of the excited level of the detector. For such tuning, there is a broad time interval where the probability of an error in detecting an excitation on the resonant qubit and distinguishing it from other excitations is smaller than that for a projective measurement by a factor ~ (γ/ΔE)², where ΔE is the difference in the qubit energies. The results bear on the scalability of quantum computers with permanently coupled qubits.
optoelectronics, and biotechnology, among other areas. The controlled, evaporative self-assembly of polymer or nanocrystal solutions yields a variety of complex, intriguing, and well-ordered structures over large confined in a simple geometry comprised of a curved surface placed upon a flat substrate. By changing the shape of the upper surface of the imposed geometry, microstructures possessing high regularity, dispensing with the need for lithographic techniques and externally applied fields. Polymer or nanocrystal solutions are sizes of high regularity and fidelity. Here, we report a facile, robust, and one-step evaporation method for producing in a precisely controllable manner versatile over the evaporation process of the drop, the challenge remains to use evaporative self-assembly to rationally “synthesize” “coffee rings” of different shapes and sizes of high regularity and fidelity. Here, we present experimentally-observed buckling morphologies resulting from a variety of surface geometries, as well as Finite Element Modeling results which provide insight into the specific evolution of stresses which led to the formation of these morphologies.

9:00AM Y18.00004 Mechanical instabilities in periodic porous elastomeric solids. We gratefully acknowledge support from NSF.

8:48AM Y18.00003 Lateral Instability of Nanoimprinted Polymer Patterns during Thermal Annealing, YIFU DING, University of Colorado, KYLIE ALVINE, Pacific Northwest National Laboratory, HYUNWOOK RO, MANISH KULKARNI, JACK DOUGLAS, CHRISTOPHER SOLES, NIST — Nanoimprint Lithography (NIL) is a promising candidate for next generation lithography. Dense polymer patterns with relatively high aspect ratios can be created using NIL. Upon thermal annealing, the as-imprinted polymer patterns will smooth out due to the surface energy and sometimes residual stress within the patterns. Both effects will predominately drive the pattern decay vertically. Here, we present that under certain patterning conditions, lateral instability of the surface patterns, driven by surface fluctuations, can also become an effective mechanism for reducing the total surface area. The characteristics of the lateral instability were successfully carried out by annealing the patterns under a temperature gradient. We demonstrate that the lateral instability can be controlled by the imprinting conditions, and can be greatly enhanced by the additions of surfactants.

8:36AM Y18.00002 Morphology of Osmotically-Driven Surface Buckles, DEREK BREID, ALFRED CROSBY, University of Massachusetts — The ordering of osmotically-driven surface buckles on an elastically-supported stiff plate depends strongly upon the dominant stresses acting on the surface during formation. For example, conditions which lead to buckle initiation at the center of the plate yield hexagonal dimple arrays characteristic of an isotropic surface stress, while buckles initiated at the edges align radially, indicating a theta-dominated state of compressive stress. Here, we work on PS-b-PEO and PS-b-PLLA shows, for the first time, the reduced tethering density value of the interacting regime transition regardless of molecular weight or solvent quality. Other factors that were not addressed include adsorption and chain stiffness effects. The work presented here will look at the role of chain adorption using miscible polymers, namely PMMA-b-PDLLA, and chain stiffness with PEO-b-PCL where PEO is the amorphous block. In addition to experimental results, Monte Carlo simulations were used to estimate the chain conformation of adsorbed PMMA.

8:12AM Y18.00005 Peculiarities in liquid phase of Styrene Butadiene rubber surface induced by Atomic Force Microscopy-assisted electrostatic nanolithography, MINDAUGAS RACKAITIS, Bridgestone Americas, SERGEI LYUKSYUTOV, The University of Akron, DMYTRO KASHYN, PAVELO PARAMONOVOV, ROBERT MALLIK — Nanoscale surface changes are reported for styrene butadiene rubber (SBR) films (100 nm) using protocol derived from Atomic Force Microscopy (AFM) electrostatic nanolithography. Under appropriate tip bias conditions, the electric field magnitude induced in SBR films is of the order of 10^8-10^9 V m^-1, which is sufficiently large to initiate cross-linking in the rubber. Peaklike surface features, surrounded by a circular trough and a raised ring, are observed after completing AFMEN-based protocol. The nanostructure dimensions vary from 0.5-20 nm high and 50-200 nm in diameter. The topology of the nanostructures is attributed to the interplay between film thickness (50 nm and thinner) and the radial component electrostatic pressure. Modeling of the electric field based on the numerical solution of Laplace equation for cylindrical geometry suggests that non-uniformity of electric field plays an important role in nanostructure formation. The stability of the features which remain stable for days suggests cross-linking between macromolecules at the nanoscale.

8:24AM Y18.00006 Diffusion-Controlled, Self-Organized Growth of Symmetric Wrinkling Patterns, CHRISTOPHER M. STAFFORD, JIN YOUNG CHUNG, ADAM J. NOLTE, Polymers Division, National Institute of Standards and Technology, POLYMERS DIVISION, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY TEAM — The formation of self-organized wrinkling patterns is a potential route for generating such tunable ordered patterns on surfaces across many length scales. Here, we demonstrate that surface wrinkling of ultraviolet/ozone (UVO) treated polymer films through osmotically driven swelling by solvent vapor sorption leads to unique and intriguing patterns, some of which have not been previously reported. The type of pattern and speed of its growth is coupled to the degree of UVO crosslinking and the rate of solvent diffusion into the film from the localized defect. This simple yet novel approach could serve as a test-bed for studying topography-driven phenomena such as wettability and adhesion and diffusion related processes, as well as facilitate a better understanding of dynamic self-assembly.

8:36AM Y18.00007 Transition from Non-interacting to Interacting Regime of Tethered Polymer Chains, RYAN VAN HORN, JOSEPH X. ZHENG, MING-SIAO HSIAO, BERNARD LOTZ, EDWIN L. THOMAS, JUTTA LUETTMER-STRATHMANN, STEPHEN Z.D. CHENG, University of Akron — Tethered polymer chains have become an important area of research over the last few decades. Their unique properties make them appealing for various applications. The tethering density of the chains determines the state of the chains as well as the resulting properties, as shown by various theoretical and experimental work. Our group uses single crystals of crystalline-amorphous diblock copolymers to study tethered polymer chains. This system provides better control of tethering density and molecular weight as compared to previous methods. Previous work on PS-b-PEO and PS-b-PDLLA shows, for the first time, the reduced tethering density value of the interacting regime transition regardless of molecular weight or solvent quality. Other factors that were not addressed include adsorption and chain stiffness effects. The work presented here will look at the role of chain adorption using miscible polymers, namely PMMA-b-PDLLA, and chain stiffness with PEO-b-PCL where PEO is the amorphous block. In addition to experimental results, Monte Carlo simulations were used to estimate the chain conformation of adsorbed PMMA.
Steric effects on the phase behavior of end-tethered temperature-responsive polymers, CHARLES HOGSHEAD, EVANGELOS MANIAS, Materials Sci & Eng; Penn State University — End-tethered polymers from a planar surface at high grafting density results in an apparent spatial confinement originating from interchain steric repulsion. This effective confinement can alter the phase behavior of temperature-responsive polymers in solution, relative to their bulk solution behavior. Here we report on experiments where we synthesized tethered polymer layers with a gradient in grafting density. The systems studied were temperature-responsive alternating copolymers in aqueous solutions. Under-water AFM was used to directly observe the tethered chain collapse upon heating through the bulk LCST, and the resulting reversible adhesion switch. The transition of the tethered layers occurs at temperatures that are similar to the binodal points of the respective solution, but over a much broader temperature range. This behavior is consistent with the collapse being a cooperative conformational transition, reflecting the effects of chain confinement, rather than a first-order thermodynamic LCST transition (as these same polymers exhibit in bulk aqueous solutions). The onset-temperature of the transition, of both the tethered layers and the LCST, was tailored by varying the copolymer composition, i.e., by tuning the hydrophilic/hydrophobic balance within the chain.

10:12 AM Y18.00010 Self-Assembling Pi-conjugated Monolayer on Silicon, J.-C. LIN, J. KELLAR, J.-H. KIM, S. NGUYEN, M. HERSAM, M. BEDZYK, Northwestern University, K. BEVAN, Purdue University — Pi-conjugated molecules play an important role in molecular electronic applications. For conductivity, the intrinsic ordering of the structure strongly influences its efficiency but is difficult to characterize by conventional scanning probe and IR spectroscopy techniques. In the present study, we combine a compliment of techniques, including XSW(X-ray standing waves), AFM, XPS, XRR(X-ray reflectivity), XRF(X-ray fluorescence), and DFT(Density functional theory) to determine the atomic scale molecular configurations and packing densities of two self-assembled aromatic monolayers (SAMs) grown on H-passivated silicon. P-4-bromophenyl-ethylphenyl-acrylene, which has two phenyl rings, is directly compared with p-4-bromophenyl-acetylene, which has only one phenyl ring. The results show a local dense packing in spite of the overall coverage being somewhat less than 0.5 monolayers. This packing of the p-4-bromophenyl-ethylphenyl-acrylene SAM suggests the average spacing between molecules is within the pi-pi interaction range, which will contribute to the charge transport. The detailed atomic structure of SAMs are also constructed using our characterization package. The result suggests the possibility of the application of self-assembling method on the growth of molecular electronics.

10:24 AM Y18.00011 The Dynamic Reinforcement of Polynvinyl Alcohol (PVA) as a Result of Non-equilibrium State of Polymer Supermolecular Structures and their Confinement in Nanofibers, EYAL ZUSSMAN, EMIL SHAKED, ARKADI ARINSTEIN, Technion — The results of mechanical testing of PVA-based electrospun nanofibers and bulk in static and dynamic modes are presented. An increase in the elastic moduli resulting from sample deformation was observed in both the bulk and as spun fibers. This increase occurs when the deformation rate exceeds a critical value and can be attributed to the non-equilibrium dynamics of the supermolecular structures of the polymer matrix. That is, the evolution of these supermolecular structures results in an observably extended relaxation time. It is noted that the rate of the modulus increase of the nanostructure is nearly double that of the bulk fibers' rate. This difference can be explained by confinement influence on the polymer matrix of the nanofibers. In addition, the tests revealed that the, Tg, of the nanofiber is noticeably higher than that of bulk specimen. Reinforcing the nanofibers by cellulose whiskers showing that the dependence of the effective modulus on the whisker concentration has an initial increase that changes to a decrease when the whisker concentration exceeds 2 %. Such behavior can be explained in the framework of an aggregation concept – when the cluster size reaches that of the fiber diameter (cluster confinement), the whisker distribution becomes inhomogeneous and results in a measurable weakening of the composite.

10:36 AM Y18.00012 Phenomenology of Polymer Thin Film Dewetting during Vapor Deposition Polymerization1, MITCHELL ANTHAMATTEN, XICHONG CHEN, University of Rochester, DEPARTMENT OF CHEMICAL ENGINEERING TEAM — Initiated chemical vapor deposition (iCVD) is a solventless technique to grow polymer thin films directly from gas phase feeds. The free radical technique involves the dissociation of gaseous initiator followed by adsorption onto a surface and subsequent polymerization with monomer to produce linear or crosslinked polymer films. We have designed and built an axisymmetric hot-zone iCVD vacuum reactor. Using this reactor, smooth poly (methyl methacrylate) polymer films are grown from methyl methacrylate and t-butyl peroxide gas feeds. When solvent vapors are added to the process, we observe dewetting of vapor deposited polymer films. The objective of the current study is to understand the phenomenology of the observed solvent-induced dewetting. White light interferometry was used to investigate the surface topography of dewetted structures. The observed length scale depends on several process parameters including the deposition rate, the type of solvent used, and the surface free energy. Higher deposition rates suppress dewetting, and higher solvent content leads to dewetted structures with larger length scales. A dynamic model is applied to explain how droplet size and droplet aerial density depend on time and process parameters.

1This study was supported by the National Science Foundation (NSF-0828437).
8:00AM Y19.00001 Sequence-directed organization in self-assembled monolayers of betapeptides on solid surfaces: A Monte Carlo simulation study. JAGANNATH MONDAL, University of Wisconsin Madison, BONG JUN, SUNG, Solagun University, ARUN YETHIRAJ, University of Wisconsin Madison — The sequence-directed organization of self-assembled monolayers (SAM) of amphiphilic β-peptides adsorbed on gold surfaces is studied using Monte Carlo simulations. A phenomenological model is considered where each (helical) molecule is represented by a rigid nano-rod with the side groups at appropriate locations. This model effectively distinguishes between two, namely globally amphiphilic (GA) and non-globally amphiphilic (non-GA), sequence-isomers of an amphiphillic β peptide Y-(ACHC-ACHC-K)1. The simulations show that the GA isomers have a high degree of orientational order that is not exhibited by the non-GA isomers, consistent with experiment. The simulations quantify a subtle balance between electrostatic, hydrophilic, and hydrophobic interactions on the self-assembly of β-peptides on surfaces. 

8:12AM Y19.00002 Thermal Response of PNIPAM Brushes Studied by Numerical Self-Consistent Field Calculations. DONG MENG, QIANG WANG, Department of Chemical and Biological Engineering, Colorado State University — Unlike most polymers, poly(N-isopropyl acrylamide) (PNIPAM) exhibits a lower critical solution temperature in water, i.e., PNIPAM chains are soluble (expand) at low temperatures and insoluble (collapse) at high temperatures. This property has been used to “smart” surfaces of PNIPAM brushes that can switch wettability, porosity and cell-adhesion properties as temperature is changed. Such thermal response of PNIPAM brushes is strongly affected by both chain length and grafting density. In this study we use numerical self-consistent field calculations with a composition-dependent Flory-Huggins parameter obtained from experiments to study the thermal response of PNIPAM brushes. The effects of chain length and grafting density are systematically investigated to provide guidance to experimental design of PNIPAM brushes for targeted applications.

8:24AM Y19.00003 Time evolution of the structure of fluorinated alkanes near solid surfaces. MESFIN TSIGE, Southern Illinois University at Carbondale — The study of thin films of physisorbed molecules has attracted much experimental and theoretical interest in the past few decades. This is mainly due to numerous reports of anomalous behavior in the structural and dynamical properties of polymeric thin films at interfaces and the expected consequences in their wide range of practical applications. Although great advances have been made in our understanding of the physics and chemistry of polymer melt/solid and polymer melt/vapor interfaces, there remain a number of fundamental as well as practical issues that need to be addressed regarding the influence of interfaces on a polymer film. One of the issues, which I think no systematic study has been yet conducted on, is the stability or time-evolution of the molecular layering in a film next to a solid surface. The main focus of my presentation will be on our recent computer simulation study result that shows that the extent of layering in an alkane film next to a solid substrate may oscillate in time with an amplitude and period that strongly depends on temperature.

8:36AM Y19.00004 Activation of CO2 on transition metal surfaces and oxide supported metal thin films. SUJATA PAUL, MARCO BUONGIORNO NARDELLI, NC State Univ — Using first principles simulations based on Density Functional Theory, we have investigated the adsorption and activation properties of CO2 on a variety of transition metal surfaces and oxide supported metal thin films. We intend to focus on the chemical conversion of CO2 through heterogeneous catalysis using surfaces and interfaces where there is nanoscale control over charge density at the reactive sites. The activation of CO2 on clean metal surfaces is possible at very high temperatures and the situation changes drastically when reaction happens on oxide supported metal thin film. The chemical reactivity of the molecule on the surface depends on the charge rearrangement at the metal-alkaline earth oxide interface. We want to understand the possible catalytic systems and characterize the relevant geometrical and electronic parameters related to the reaction mechanisms, rates and yield.

8:48AM Y19.00005 Dynamics of an Adsorbed Polymer Chain. JOSHUA KALB, SANAT KUMAR, Columbia University — Because of the current precision in fluorescent labeling, it is possible to label single polymers such as DNA or PEG and track their dynamical and equilibrium properties in the bulk as well as near attractive surfaces [Maier et. al., Macro. 2000][Sukhishvili et. al., Macro. 2002]. Recent evidence from these experiments and related simulations has shown that the dynamics of a single polymer near an attractive surface appear diffusive, however further evidence coming from the ‘diffusion coefficient’ implies a different process other than diffusion is at work such as reptation, ‘hover crafting’, or ‘hopping’ [Sukhishvili et. al., Macro. 2002]. In general, these possible dynamical behaviors are determined by the length of the polymer itself as well as the microscopic details of the attractive surface which include the density, strength, and distribution of attractive surface sites[Desai et. al., PRL 2007][Qian et. al., PRL 2007]. In this presentation, we investigate the effects of microscopic surface sites on single polymer dynamics through DMD simulations and compare these results to the properties of the chain in the bulk and near a flat attractive surface.

9:00AM Y19.00006 Investigation of Carboxymethyl Cellulose Adsorption onto Regenerated Cellulose Surfaces via Quartz Crystal Microbalance with Dissipation Monitoring and Surface Plasmon Resonance Spectroscopy. ZELIN LIU, Department of Chemistry (0212), Virginia Tech, Blacksburg, VA 24061, PAUL GATENHOLM, Department of Materials Science and Engineering (0237), Virginia Tech, Blacksburg, VA 24061, ALAN ESKER, Department of Chemistry (0212), Virginia Tech, Blacksburg, VA 24061 — The adsorption of anionic polyelectrolytes, sodium salts of carboxymethyl celluloses (CMC), with different degrees of substitution (DS = 0.9 and 1.2) from aqueous electrolyte solutions onto regenerated cellulose surface was studied via quartz microbalance with dissipation monitoring (QCM-D) and surface plasmon resonance (SPR) spectroscopy. The adsorption of CMC (100 mg L−1) from 0.1 M sodium chloride (NaCl) was examined. Both QCM-D and SPR results indicate that CMC adsorption onto regenerated cellulose surfaces increases with increasing electrolyte concentration and CaCl2 (diluent) showed a significant effect on CMC adsorption compared to NaCl (monovalent cation) at the same ionic strength. Voigt-based viscoelastic modeling of the QCM-D data and analysis of the SPR data are consistent with the existence of a swollen CMC layer on the cellulose surface with a viscosity of ~1.310−3 kg m−1 s−1 and an elastic shear modulus of ~105 kg m−1 s−2.

9:12AM Y19.00007 Theory of Polymer Adsorption Onto Selected Chemically Patterned Substrates. ALEXANDER CHERVANYOV, GERT HENRICH, Leibniz Institute of Polymer Research Dresden — We theoretically studied the reversible adsorption of polymers onto selected rigid and soft chemically non-uniform substrates with an emphasis on the polymer adsorption onto the selective binary mixed brushes. In the course of our study, we developed two independent theoretical methods, the self-consistent perturbation expansion and the transfer operator formalism, which made it possible to thoroughly investigate the density structure of polymers adsorbed onto chemically non-uniform substrates. As successive stages of our research, we applied the above theoretical methods to the study of the polymer adsorption onto the selected substrates, as follows: (i) periodically patterned rigid surface; (ii) randomly patterned rigid surface; (iii) surface that bears an array of periodically distributed adsorption centers; (iv) ripple, random and dimple morphologies of the binary mixed brush. By comparing the results obtained for the above listed systems we derived the qualitative trends that are common for the polymer adsorption onto the investigated chemically non-uniform substrates. In this talk, we discuss what are the main factors that influence the polymer adsorption onto the patterned substrates and how to reduce/enhance the polymer adsorption by way of manipulating these competitive factors.
Tunable Sliding Angles from isotactic-Polypropylene / Polypropylene Chloride Blend

XIA DONG, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Sciences, SONG HONG, YONGHUA YAO — With proper selection of shear and thermal conditions, super-hydrophobic polymeric surfaces (Contact angle higher than 150°) with tunable sliding angles (From less than 1° to higher than 90°) can be prepared from isotactic polypropylene (iPP)/ polypropylene chloride (PPC) blend under ambient atmosphere. No further modification with low-surface-energy component is needed. The formed surfaces have good thermal property, chemical and moisture resistance and potentially low manufacturing cost.

Joint Laboratory of Polymer Science and Materials, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China

Friday, March 20, 2009 8:00AM - 10:36AM –
Session Y20 DPOLY: Biological-Synthetic Hybrid Materials

8:00AM Y20.00001 Peptide Folding and Consequent Self-assembly for Shear Thinning Hydrogels with Immediate Recovery

DARRIN POCHEK, University of Delaware — The local nano- and overall network structure, and resultant viscoelastic properties, of hydrogels that are formed via beta-hairpin self-assembly will be presented. The 20 amino acid peptides have been shown to intramolecularly fold and intermolecularly self-assemble into a rigid hydrogel based on environmental cues such as pH, salt, and temperature including physico-chemical conditions. The hydrogel is composed of a network of fibrils that are 3 nm wide that physically crosslink (i.e. entangle and branch) with no covalent crosslinking required. Slight design variations of the peptide sequence allow for tunability of the self-assembly/hydrogelation kinetics. In turn, by controlling hydrogel self-assembly kinetics, one dictates the ultimate stiffness of the resultant network. This physical assembly process allows the encapsulation of desired payloads into the gel network such as large macromolecules or living cells. Importantly, once formed into a solid, the self-supporting gel network can be disrupted by the introduction of a shear stress. The system can shear thin but immediately heal to a stiff solid on the cessation of the shear stress. This shear thinning and recovery behavior makes them interesting candidates for injectable delivery in vivo.

In collaboration with Joel Schneider, University of Delaware.

8:36AM Y20.00002 Designing ‘smart’ hydrogels using peptide-responsive conjugates

ALBERTO SAIJANI, JEAN-BAPTISTE GUIBAUD, ALINE MILLER, The University of Manchester — Polymers displaying phase transitions in aqueous solution from a hydrophobic to hydrophobic state are of widespread interest as ‘smart’ biomedical materials. Hydrogels formed from self-assembling peptides have also attracted considerable attention in the past decade. These hydrogels are based on the self-assembly of short peptides into supra-molecular fibres that entangle or associate to form three dimensional networks and, ultimately, self-supporting hydrogels. In order to create a new generation of hydrogel based on self-assembling peptides but possessing an internal transition that can be used as a trigger to release a drug molecule or a specific biological signal we have synthesized a new family of peptide-polymers conjugates using free radical polymerization. We were able to create a new generation of ‘smart’ hydrogel in which gelation is driven by the peptide while the polymer phase transition can be used to release in a controlled fashion a specific signal or drug molecules. These materials are though to be of prime interest for tissue culture applications where they can be used to deliver specific signals stimulating a specific cell response.

In collaboration with Joel Schneider, University of Delaware.

8:48AM Y20.00003 “Backpack” Functionalized Living Immune Cells

ALBERT SWISTON, MIT Dept of Materials Science and Engr., SOONG HO UM, DARRELL IRVINE, MIT Dept of Biological Engr., ROBERT COHEN, MIT Dept of Chemical Engr., MICHAEL RUBNER, MIT Dept of Materials Science and Engr. — We demonstrate that functional polymeric “backpacks” built from polyelectrolyte multilayers (PEMs) can be attached to a fraction of the surface area of living, individual lymphocytes. Backpacks containing fluorescent polymers, superparamagnetic nanoparticles, and commercially available quantum dots have been attached to B and T-cells, which may be spatially manipulated using a magnetic field. Since the backpack does not occlude the entire cellular surface from the environment, this technique allows functional synthetic payloads to be attached to a cell that is free to perform its native functions, thereby synergistically utilizing both biological and synthetic functionalities. For instance, we have shown that backpack-modified T-cells are able to migrate on surfaces for several hours following backpack attachment. Possible payloads within the PEM backpack include drugs, vaccine antigens, therapeutically responsive polymers, nanoparticles, and imaging agents. We will discuss how this approach has broad potential for applications in bioimaging, single-cell functionalization, immune system and tissue engineering, and cell-based therapeutics where cell-environment interactions are critical.

This work was supported primarily by the MRSEC Program of the NSF under award number DMR-0819762, and is based upon work supported by a NSF Graduate Research Fellowship.

9:00AM Y20.00004 Reversible Structural Transition of a DNA Lipid Film

MATTHEW TIRRELL, SUREKHA GAJRIA, THORSTEN NEUMANN, LUC JAEGE, University of California, Santa Barbara, MATERIALS RESEARCH LABORATORY COLLABORATION — Polyanions such as nucleic acids (RNA and DNA) can self-assemble with cationic lipids via electrostatic complexation, driven thermodynamically by the release of counterions. The structures of these complexed films in water have been studied extensively and are recognized as potentially useful in the field of gene delivery. The structure of films in water is dominated by the nature of the lipid. Within these lamellar complexes in aqueous solution the lipid assumes a bilayer formation and the DNA is a double helix. It is possible to obtain dry nucleic acid lipid films when the dissolved cationic lipid complex of DDAB and nucleic acid is cast on a solid. These self-standing films have been characterized by tensile properties and nucleic acid intercalation experiments. The tensile properties of these films are adjustable by mixing different molecular weights. It was expected that these films would have the same characteristic structure as these complexes in water. However, our work shows that the film undergoes a transition from double stranded helical DNA complexed with a bilayer of DDAB in the wet state, while in the dry state we observed a repeat unit of single stranded DNA complexed with a monolayer of DDAB.

9:12AM Y20.00005 Gecko-Inspired Carbon Nanotube-Based Adhesives

LIEHUI GE, SUNNY SETHI, ANUBHA GOYAL, LIJIE CI, PULICKEL AJAYAN, ALI DHINOJWALA, THE UNIVERSITY OF AKRON COLLABORATION, RICE UNIVERSITY COLLABORATION — Nature has developed hierarchical hair structure on the wall-climbing gecko’s foot, consisting of microscopic hairs called setae, which further split into hundreds of smaller structures called spatulas. In the last five years, numerous attempts to mimic gecko foot hair using polymer soft molding and photolithography methods have been reported. However, most of these polymer-based synthetic gecko hairs fall short of the clinging ability of geckos. Vertically aligned carbon nanotubes (CNT) have shown strong adhesion at nanometer scale. Here, we present our work on developing CNT-based macroscopic flexible tape mimicking the hierarchical structure found on gecko’s foot. The synthetic gecko tape is made by transferring aligned CNT array onto flexible polymer tape. The unpatterned CNT-gecko tape can support a shear force stress similar to gecko foot (10 N/cm²). The supported shear stress increase by a factor of four, when we use micro-patterned CNT patches (50 to 500 μm). We find that both setae (replicated by CNT bundles) and spatulas (individual CNT) are necessary to achieve large macroscopic shear adhesion. The carbon nanotube-based tape offers an excellent synthetic option as a dry conductive reversible adhesive in microelectronics, robotics, and space applications.

Research Supported by National Science Foundation
the results of recent experiments to hyperpolarize the nuclear spins can be a significant limitation, whether the nuclear spins are used as qubits or act as an environment for the electronic spins. We report the

DNA:Ag visible excitation, suggesting energy transfer from the DNA bases to the Ag cluster. We make use of this UV excitation to image the emitters in unstained wavelengths for all DNA-bound Ag clusters. This UV peak corresponds to resonant absorbance by the DNA bases, and produces the same emission spectra as a ubiquitous feature of these emitters. Each emitter thus has two excitation peaks: a visible peak which is cluster-dependent, and a UV peak which has the same

KIM WEIRICH, DEBORAH FYGENSON, University of California Santa Barbara — Few-atom fluorescent Ag nanoclusters self-assemble on short, synthetic micropatterned surface layers of two different proteins: silk fibroin (for growth of gold and silver nanoparticles) and silaffin (for growth of titania nanoparticles). We demonstrate that all titania, gold, and silver nanoparticles can be grown with relatively monodisperse diameter within 4-6 nm surrounded by biological shells of 1-2 nm thick. As biological templates we utilized ultrathin, molecular uniform and inorganic nanoparticles at room temperature and ambient conditions. We will discuss possible preferential chain conformations that may provide the driving force for the superstructure.

9:48AM Y20.00008 The effects of supramolecular network topology on hapten-receptor avidity . JASON BENKOSKI, ANDREW MASON, JILL LA FAVORS, JOSHUA WOLFE, The Johns Hopkins University Applied Physics Laboratory — Antibodies produced in the early stages of the immune response have much lower affinities for a given antigen than those produced later on. Nature compensates for the initial weakness of these associative bonds by synthesizing multivalent antibodies. The total binding strength, represented by the avidity constant, is equal to the product of the affinity constants for the individual hapten/receptor sites. However, under realistic conditions the individual binding sites do not act independently. Factors such as steric hindrance, intramolecular stresses, and competitive binding can significantly alter the relationship between affinity and avidity. We investigate the influence of these factors on a model system consisting of synthetic multifunctional nanoparticles and polymers. Each polymer or nanoparticle is decorated with either multiple antigens (thromboxane B2) or multiple antibodies. We then measure the association and dissociation in real time using Surface Plasmon Resonance Spectroscopy (SPR). By using synthetic polymers and nanoparticles, we are able to systematically control the degree of functionality, flexibility, and distance between receptor and hapten sites.

10:00AM Y20.00009 Dynamic DNA Interactions with Functionalized Colloids , LU ZHANG, YINGXI ELAINE ZHU, Department of Chemical and Biomolecular Engineering, University of Notre Dame — Many biomedical processes, such as protein adsorption, DNA hybridization and enzyme reactivity, are intimately related to their interactions with surfaces and complex ionic environments, yet the details of biomacromolecular interaction remain insufficiently understood. In this work, we use confocal laser scanning microscopy to examine the interaction between DNA molecules and functionalized colloidal particles in aqueous suspension. We observe an intriguing attractive interaction between DNA molecules and carboxyl-functionalized silica particles of varied sizes from 50 nm to 3 um, resulting in complex DNA-colloid aggregation with a strong dependence on DNA/colloid size ration and ionic strength. As colloidal size becomes larger than DNA dimensions, colloidal doublets and triplets with adsorbed DNAs are observed at high DNA concentration and ionic strength. The intriguing DNA-colloid complex structures are further confirmed by SEM and appear stable for at least 2 weeks.

10:12AM Y20.00010 Growth of well-defined metal and oxide nanoparticles on biological surfaces . VLADIMIR TSUKRUK, Georgia Tech — We present a brief overview of our recent studies in the field of bio-enabled surface-mediated growth of inorganic nanoparticles at room temperature and ambient conditions. We demonstrate that all titania, gold, and silver nanoparticles can be grown with relatively monodisperse diameter within 4-6 nm surrounded by biological shells of 1-2 nm thick. As biological templates we utilized ultrathin, molecular uniform and micropatterned surface layers of two different proteins: silk fibroin (for growth of gold and silver nanoparticles) and silaffin (for growth of titania nanoparticles). To identify the grown nanophases and chemical composition/secondary structure of biological templates we applied combined AFM, SEM, TEM, XPS, SERS, UV-vis, and ATR-FTIR techniques.

10:24AM Y20.00011 Fluorescent DNA-bound Ag nanoclusters , PATRICK O’NEILL, LOURDES VELAZQUEZ, KIM WEIRICH, DEBORAH FYGENSON, University of California Santa Barbara — Few-atom fluorescent Ag nanoclusters self-assemble on short, synthetic DNA strands, and exhibit sequence and structure dependent fluorescence ranging from the blue to the near infrared. Here we report UV excitation as a ubiquitous feature of these emitters. Each emitter thus has two excitation peaks: a visible peak which is cluster-dependent, and a UV peak which has the same wavelength for all DNA-bound Ag clusters. This UV peak corresponds to resonant absorbance by the DNA bases, and produces the same emission spectra as a visible excitation, suggesting energy transfer from the DNA bases to the Ag cluster. We make use of this UV excitation to image the emitters in unstained polyacrylamide gels, and show that electrophoresis can be used to create a pure solution of green DNA:Ag11 clusters from an inhomogeneous red solution of DNA:Ag>12 clusters.

Friday, March 20, 2009 8:00AM - 10:48AM
Session Y22 GMAG DMP FIAP: Focus Session: Spin Resonance in Semiconductors 324

8:00AM Y22.00001 Dynamic Nuclear Polarization in Silicon . CHANDRASEKHAR RAMANATHAN, Massachusetts Institute of Technology — Silicon is a promising material for spintronics and spin-based quantum information processing. However, the highly mixed state of the nuclear spins can be a significant limitation, whether the nuclear spins are used as qubits or act as an environment for the electronic spins. We report the results of recent experiments to hyperpolarize the 29Si spins in silicon. We used microwave-induced dynamic nuclear polarization to achieve 5% polarization of the 29Si in micro-crystalline silicon powder [1], and 5–8% polarization in antimony- and phosphorus-doped silicon wafers. Since silicon has long T1 relaxation times, polarized silicon micro- and nanoparticles could be of use in magnetic resonance imaging. In the powders the 29 Si nuclei in the amorphous region (containing unpaired electrons) are polarized by forced electron-nuclear spin flips driven by off-resonant microwave radiation while nuclei in the crystalline region are polarized by spin diffusion across crystalline boundaries. In the wafers the DNP is driven by an Overhauser mechanism within exchange-coupled clusters of donors.

AMRIT DE, CRAIG E. PRYOR, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — The orbital wave function of an electron

currently by the experimental setup. This shows that this method has the expected high bandwidth opening the view to faster phenomena in EDMR in a more

bandwidth by using frequency modulation of the microwaves applied indicates that the spin signature observed with the tank circuit is limited at the high end

current preamplifier and in-situ by the response of the LRC resonant circuit and observe a spin resonance signature in both cases. Investigating the detection

the sample in a LRC resonant circuit, a so-called tank circuit, it is possible to overcome this limitations. Here, we investigate a silicon MOSFET where the

Typically, the detection bandwidth of EDMR is limited by the characteristic RC time constant of the sample. In this contribution we show that by embedding

realization of quantum computation with the help of the spin degree of freedom in semiconductors. Electrically detected magnetic resonance (EDMR) provides

theoretical simulations have the potential to reveal information about spin polarization and electronic structure of bulk semiconductors with far greater sensitivity

with theoretical calculations, we have mapped out the conduction band electronic spin polarization. We show that OPNMR experiments in combination with

experiments resolve fine details of the spin-dependent electronic structure of the valence bands. By comparing the oscillations in the OPNMR signal intensity

and the spin splitting can be observed in the circularly polarized magneto-absorption spectra. By carefully analyzing the energy band structure and the absorption

experiments. Although GaAs has a small $g$-factor leading to nearly spin-degenerate conduction band Landau levels, the valence band Landau levels are spin-split

and the spin splitting can be observed in the circularly polarized magneto-absorption spectra. By carefully analyzing the energy band structure and the absorption

spectra together, we identify the origins of all the optical transitions. We also separate contributions to the absorption coefficient from spin-up electrons and

spin-down electrons to get the conduction band electron spin polarization. This information is used to compute the optically-pumped NMR (OPNMR) signal.

We demonstrate that OPNMR can provide unique insight into the spin-dependent valence band electronic states.

1Supported by NSF through Grants: CHE- 0239560, DMR 0706313, and INT 0530220, and through I-CARES, Washington Univ.

2This work was supported by the Office of Naval Research and NSF under DMR 08-04244.

8:48AM Y22.00003 Electric-field control of a hydrogenic donor’s spin in a semiconductor1 .

AMRIT DE, CRAIG E. PRYOR, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — The orbital wave function of an electron

bound to a single donor in a semiconductor can be modulated by an applied AC electric field, which affects the electron spin dynamics via the spin-orbit

interaction. Numerical calculations of the spin dynamics of a single hydrogenic donor (Si) using a real-space multi-band $k$-$p$ formalism show that in addition to

breaking the high symmetry of the hydrogenic donor state, the $g$-tensor has a strong nonlinear dependence on the applied fields. By explicitly integrating the

time dependent Schrödinger equation it is seen that Rabi oscillations can be obtained for electric fields modulated at sub-harmonics of the Larmor frequency.

The Rabi frequencies obtained from sub-harmonic modulation depend on the magnitudes of the AC and DC components of the electric field. For a purely AC

field, the highest Rabi frequency is obtained when E is driven at the 2nd sub-harmonic of the Larmor frequency. Apart from suggesting ways to measure $g$-tensor

anisotropies and nonlinearities, these results also suggest the possibility of direct frequency domain measurements of Rabi frequencies.

3C.E.P. would like to acknowledge an NSF NIRT. M.E.F. would like to acknowledge an ONR MURI.

8:00AM Y22.00004 Electronic spin polarization and spin-dependent band structure in GaAs

probed by optically-pumped NMR (OPNMR)1 . SOPHIA HAYES, KANANN RAMASWAMY, STACY MUI, Washington U., SCOTT CROOKER, NHMF, Los Alamos, XINGYUAN PAN, GARY SANDERS, CHRISTOPHER STANTON, Univ. of FL — Traditionally, magnetic fields have played an important role in determining the band structure of a material (de Haas-van Alphen techniques for metals and cyclotron resonance or magneto-

absorption for semiconductors). We report optically pumped NMR (OPNMR) spectra of 69Ga spins in bulk semi-insulating GaAs generated by a narrowband

laser. OPNMR involves optical orientation of electrons in a semiconductor with NMR detection of the polarized nuclear spins to which they are coupled. These

experiments resolve fine details of the spin-dependent electronic structure of the valence bands. By comparing the oscillations in the OPNMR signal intensity

with theoretical calculations, we have mapped out the conduction band electronic spin polarization. We show that OPNMR experiments in combination with

theoretical simulations have the potential to reveal information about spin polarization and electronic structure of bulk semiconductors with far greater sensitivity

than conventional techniques such as magneto-absorption.

1Supported by NSF through Grants: CHE- 0239560, DMR 0706313, and INT 0530220, and through I-CARES, Washington Univ.

9:12AM Y22.00005 Theory of the Spin-Splitting of the Valence Band Landau Levels in GaAs1


High Magnetic Field Laboratory — We present calculations of the spin-dependent band structure and magneto-optical absorption spectra in bulk GaAs.

Our calculations are based on the 8-band Pidgeon-Brown model. Optical properties are calculated within the golden rule approximation and compared with

experiments. Although GaAs has a small $g$-factor leading to nearly spin-degenerate conduction band Landau levels, the valence band Landau levels are spin-split

and the spin splitting can be observed in the circularly polarized magneto-absorption spectra. By carefully analyzing the energy band structure and the absorption

spectra together, we identify the origins of all the optical transitions. We also separate contributions to the absorption coefficient from spin-up electrons and

spin-down electrons to get the conduction band electron spin polarization. This information is used to compute the optically-pumped NMR (OPNMR) signal.

We demonstrate that OPNMR can provide unique insight into the spin-dependent valence band electronic states.

1Supported by NSF through Grants: CHE- 0239560, DMR 0706313, and INT 0530220, and through I-CARES, Washington Univ.

9:24AM Y22.00006 High bandwidth EDMR detection , H. HUEBL, L.H. WILLEMS VAN BEVEREN, R.P. STARRETT, D.R. MCCAMEY, A.J. FERGUSON, Centre for Quantum Computer Technology, University of New South Wales, Sydney — Several proposals discuss the realization of quantum computation with the help of the spin degree of freedom in semiconductors. Electrically detected magnetic resonance (EDMR) provides a well established tool to investigate spin states in semiconductors which was recently extended to investigate the spin dynamics of phosphorus donors in silicon.

Typically, the detection bandwidth of EDMR is limited by the characteristic RC time constant of the sample. In this contribution we show that by embedding

the sample in a LRC resonant circuit, a so-called tank circuit, it is possible to overcome this limitations. Here, we investigate a silicon MOSFET where the

microwave magnetic field to induce the spin transitions is generated on chip by a shorted coplanar stripline[1]. We monitor the MOSFET resistance with a current

preamplifier and in-situ by the response of the LRC resonant circuit and observe a spin resonance signature in both cases. Investigating the detection

bandwidth by using frequency modulation of the microwaves applied indicates that the spin signature observed with the tank circuit is limited at the high end

currently by the experimental setup. This shows that this method has the expected high bandwidth opening the view to faster phenomena in EDMR in a more

direct manner. [1] Willems van Beveren et al., APL 93, 072102 (2008)

9:36AM Y22.00007 Optically Detected Electron Spin Resonance of GaAs Spin-LEDs , JOHN COLTON, STEVE BROWN, BENJAMIN HEATON, DANIEL JENSON, MICHAEL JOHNSON, AARON JONES, Brigham Young University — GaAs “spin-

LED” samples give off circularly polarized light due to spin-polarized electrons being injected into a quantum well diode structure. The spin dynamics of these

electrons have been studied through electron spin resonance (ESR), with the resonance being optically detected by a change in the circular polarization of the

emitted light. Results of the ESR experiments will be presented.
9:48AM Y22.00008 Spin lifetime properties of a quantum well GaAs sample measured by optically detected magnetic resonance \(^1\), BENJAMIN HEATON, JOHN COLTON, STEVE BROWN, DANIEL JENSON, MICHAEL JOHNSON, AARON JONES, Brigham Young University — Optically detected Kerr rotation techniques were used to measure spin properties in GaAs. The samples studied were MBE-grown 14 nm n-type GaAs quantum wells. Magnetic resonance was observed with high sensitivity as the probe laser was tuned to the exciton resonance. The g-factor was measured to be \(|g|=0.35\). The \(T_1\) lifetime measured from the width of the ODMR peaks was 52 ns. Results from pulsed microwave Rabi oscillation and spin echo experiments (to measure the \(T_2\) spin coherence lifetime) are presented.

\(^1\)This work was supported by NSF grants 0419501, 0456074, and 0802831.

10:00AM Y22.00009 Ballistic Spin Resonance, SERGEY FROLOV, SILVIA LUESCHER, WING-WA YU, YUAN REN, JOSHUA FOLK, UBC, WERNER WEIGSCHIEBER, University of Regensburg — We demonstrate spin resonance driven by ballistic motion of electrons and mediated by spin-orbit interaction in a micron-scale channel of GaAs/AlGaAs two-dimensional electron gas. The resonance is observed when the frequency of electron bouncing trajectories in the channel matches the spin precession frequency set by a large in-plane magnetic field. The resonance is manifested as a suppression of pure spin currents that are generated in the channel by injection through quantum point contacts. The resonant frequency (10-50 GHz) can be tuned by varying electron density or channel width, as well as by bending the electron trajectories with a small out-of-plane magnetic field.

10:12AM Y22.00010 Scaling behavior of spin-dependent scattering off Neutral Donors in Silicon Field-Effect Transistors \(^1\), C. C. Lo, J. BOKOR, University of California, Berkeley, T. SCHENKEL, Lawrence Berkeley National Laboratory, J. HE, A. M. TYRYSHKIN, S.A. LYON, Princeton University — Spin-dependent scattering of conduction electrons by neutral impurities is a promising route towards donor nuclear spin-state readout for donor qubits in silicon. Using electron spin resonance techniques, the donor nuclear spin-state can be extracted from the position of the resonance signal. Contrary to readout schemes involving Coulomb/spin blockade or other single electron phenomenon, spin-dependent scattering can be observed and studied in the presence of an ensemble of donors. In our experiments we study neutral impurity scattering of two-dimensional conduction electrons by donor impurities in field-effect transistors [1]. In this talk, we will discuss the scaling behavior of donor resonance signals using electrically detected magnetic resonance techniques in devices with different sizes. [1] C. C. Lo et al, App. Phys. Lett., 91, 242106 (2007)

1Supported by the National Security Agency and the U.S. Department of Energy under contract no. DE-AC02-05CH11231.

10:24AM Y22.00011 Electron Spin Resonance in Si/SiGe Heterostructures at 350 mK \(^1\), JIANHUA HE, A.M. TYRYSHKIN, S.A. LYON, Princeton University, D.E. SAVAGE, M.A. ERIKSSON, University of Wisconsin-Madison — Si/SiGe heterostructures are one of the promising matrices for electron spins as qubits in a silicon-based quantum computer. Many electron spin resonance (ESR) measurements have been done to characterize 2D electron spins embedded in such structures at temperatures above 2 K. Here we report the first CW and pulsed ESR experiments in Si/SiGe heterostructures in a \(^3\)He system at 350 mK. Electron beam lithography was used to pattern a large area (16 mm\(^2\)) of a CVD grown modulation doped Si/SiGe quantum well (QW) into an array of \(\sim 100 \) nm quantum dots (300 nm pitch) which has been wet etched about half-way through the doped layer. In the dark, only one signal is observed, which shows a Curie-like temperature dependence indicative of isolated spins. After brief illumination, two more signals appear: a line having g-factor \(g = 0.19\) and another line which disappears upon annealing to 20 K. The first of these lines \((g = 2.0003)\) shows a Pauli temperature dependence consistent with many-electron quantum dots, and a \(T_2\) relaxation time of about 150 ns at 350 mK. The origin of these ESR signals and their relaxation mechanisms will be discussed.

1Supported by LPS/ARO.

10:36AM Y22.00012 Electron spin resonance in silicon MOS structures down to 0.36 K \(^1\), S. SHANKAR, A. M. TYRYSHKIN, S. A. LYON, Princeton University — While transport of 2-dimensional (2D) electrons has been routinely measured down to few mK, performing electron spin resonance (ESR) at low temperatures is challenging. We report measurements of the paramagnetic susceptibility of 2D electrons in a silicon metal-oxide-semiconductor (MOS) structure using ESR at 0.34 T for temperature down to 0.36 K. When the MOS gate is biased below the threshold voltage, we measure electrons weakly confined below the conduction band edge and find that the susceptibility follows a simple Pauli temperature dependence, i.e., constant at low temperatures. Surprisingly, at an electron density of \(2.8 \times 10^{11} \text{ cm}^{-2}\) (Fermi temperature \(= 20 \text{ K}\), as the temperature is reduced from 4.2 K to 0.36 K, the susceptibility actually drops by a factor of 2. Furthermore, this effect becomes more pronounced at higher 2D electron densities. The drop in susceptibility for 2D conduction electrons at low temperature is unexpected and remains to be explained.

1Supported by LPS/ARO.

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Friday, March 20, 2009 8:00AM - 10:48AM – Session Y24 DMP: Focus Session: Hydrogen Storage: Atomic and Molecular Motions 326

8:00AM Y24.00001 Atomic Motions in Ionic Hydrides: MgH\(_2\), NaMgH\(_3\), and LiBH\(_4\), MARK CONRADI, Washington University — In hydrogen storage, rapid hydrogen diffusion is a key component for rapid reaction rates of dehydriding and rehydriding. In metallic systems, the light interstitial H atoms typically do display rapid diffusion. However, recent interest has focused on ionic and complex hydrides of light metal-atoms because of their high weight fractions of reversible hydrogen. These ionic complex hydrides generally reveal slow hydrogen diffusion and resulting slow reaction kinetics. We report here studies of H diffusion using NMR in several such hydrides. In MgH\(_2\), the rate \(\omega_H\) of H hopping remains too slow to narrow the H NMR up to 400 °C. T\(_{1D}\) measurements, however, can detect the motion and find an activation energy of 1.72 eV, the first reported direct measurement of diffusion in MgH\(_2\). In ball-milled (bm) material with Nb\(_5\) catalyst additive, a fraction of the resonance intensity is narrowed starting at 50 °C, with the narrow fraction growing up to 30% by 400 °C. A model for continuous growth of the narrow line, based on a wide distribution of motion rates, is presented. Ball-milling also greatly increases the laboratory-frame relaxation rates, \(T_1^{-1}\), from paramagnetic defects created by the mechanical process. In bm NaMgH\(_3\), an even larger fraction of the resonance is motionally-narrowed, growing to nearly 100% by 300 °C. Clearly, ball-milling has a much more profound effect on ionic hydrides than the simple reduction of grain sizes and diffusion distances. In coarse-grain LiBH\(_4\) (with 13.8 weight%) reversible hydrogen), an orientationally disordered solid phase occurs above 110 °C. Above the transition, the rate of Li ion diffusion increases remarkably. H diffusion starts to narrow the H NMR line around 170 °C, continuing to narrow up to the melt near 280 °C. To distinguish diffusion of (already rapidly rotating) BH\(_4\) units from H exchange between neighboringBH\(_4\), the \(2^1\)B resonance was studied. The boron line central transition becomes much narrower (400 Hz) than the width (1500 Hz) expected from Van Vleck M\(_2\) for the case of static boron spins (with rapid Li and H diffusion). Thus, intact BH\(_4\) units are the diffusing species. Even in molten LiBH\(_4\), the BH\(_4\) lifetime is found to be at least 2 seconds from observations of the B-H J-coupling pattern, so it is probably much larger in the solid.
8:36AM Y24.00002 Understanding and Enhancing Hydrogen Diffusion in MgH2 and NaMgH3, DAVID SHOLL, SHIQIANG HAO, Georgia Tech — The transport properties of hydrogen in metal hydrides are crucial to the kinetics of H2 storage in these materials. We use first-principles calculations to identify the defects that are relevant for H transport in MgH2 and NaMgH3. In both materials, the physically relevant defects are charged and diffusion is dominated by mobility of negatively charged interstitial H. Interestingly, the diffusion of these species occurs via concerted mechanisms with low energy barriers. To improve the charged interstitial H diffusivity, a series of transition-metal additives are screened to lower the formation energy of mobile defects. Our results provide a practical way to examine and alter H diffusion in light metal hydrides.

8:48AM Y24.00003 Quasielastic Neutron Scattering of Hydrogen Adsorbed in KC24, JUSTIN PUREWAL, JAMES KEITH, CHANNING AHN, BRENT FULTZ, California Institute of Technology, CRAIG BROWN, NIST Center for Neutron Research — Quasielastic neutron scattering (QENS) and volumetric techniques were used to study the adsorption of H2 by the stage-2 potassium graphite intercalation compound KC24. A zero-coverge sorption enthalpy of 8.5 kJ/mol was measured from H2 isotherms recorded at 77 K and 87 K. The saturation H2 adsorption amount at 77 K was 1.2 mass%, corresponding to a stoichiometry of KC24/(H2)2/0. Quasielastic neutron scattering spectra for KC24/(H2)1/0 were collected at temperatures between 40 K and 80 K on a chopper spectrometer and a backscattering spectrometer. Two distinct H2 diffusion processes were identified with characteristic times of approximately τ = 10 ps and τ = 350 ps at 60 K, respectively. By operating the backscattering spectrometer in fixed window mode, the total elastic scattering of KC24/(H2)1/0 was measured as a function of temperature. A sharp decrease in elastic intensity was observed at 35 K due to the onset of quasielastic scattering. This was interpreted as a melting transition of the H2 adsorbate in KC24.1 This work was supported by the Office of Energy Efficiency and Renewable Energy through the Hydrogen Sorption Center of Excellence.

9:00AM Y24.00004 Novel geometry for simultaneous resistive, Hall and optical measurement of MgH2 thin films, D.W. KOON, C. C. W. GRIFFIN, St. Lawrence University, J.R. ARES, F. LEARDINI, C. SANCHEZ, Universidad Autónoma de Madrid — We describe a novel specmen geometry that we have used to simultaneously probe optical transmission, sheet resistance and sheet Hall resistance in 100 nm Mg films during hydrogen absorption. A Mg-film cloverleaf overlaps four rectangular Pd pads at the corners of a glass slide, a variation on a two-pad geometry used by Ingason and Olafsson for resistive studies of Pd-capped MgH2 films [J. Alloys and Compounds 404–406 (2005), 469–72]. Hydrogen diffuses laterally through the Pd pads before entering the magnesium layer from below. The sample holder also includes an LED-photodiode pair for measuring [monochromatic] optical transmission. We show that the simultaneous measurement of these three quantities during the metal-to-insulator transition in a hydriding MgH2 film allows for a more complete understanding of the hydriding process in these films.

9:12AM Y24.00005 Proton Tunneling: A Decay Channel of the O-H Stretch Mode in KTaO3, ERIK SPAHR, College of William and Mary, MICHAEL STAVOLA, Lehigh University, LANLIN WEN, Lehigh University, LYNN BOATNER, Oak Ridge National Lab, LEONARD FELDMAN, Vanderbilt, Rutgers, NORMAN TOLK, GUNTER LUPKE, College of William and Mary — Proton vibrational dynamics play a key role in the important processes of hydrogen diffusion and transport. In particular, perovskite structured proton conductors are an important class of hydrogen transport materials with a wide range of applications. We have measured for the first time the vibrational lifetimes of the O-H and O-D stretch modes in the perovskite oxide, KTaO3, by pump-probe infrared spectroscopy. Both stretch modes are exceptionally long lived and exhibit a large “reverse” isotope effect, due to a phonon-assisted proton tunneling process, which involves the O-Ta-O bending motion. The excited-state tunneling rate is found to be seven orders of magnitude larger than that in the ground state in the proton conducting oxide, BaCeO3 [1]. [1] I. Kuskovskiy et al., Phys. Rev. B 60, R3713 (1999).

9:24AM Y24.00006 Reversible Low Temperature Hydrogen Storage Using Ternary Borides, WEN LI, JOHN VAJO, ROBERT CUMBERLAND, PING LIU, HRL Laboratories, LLC, SÔN-JONG HWANG, CHUL KIM, California Institute of Technology, ROBERT BOWMAN, RCB Hydrides, LLC — Among many materials for hydrogen storage, complex borohydride of light metals with high hydrogen capacity, have been studied extensively. However, the thermodynamic and kinetic properties of borohydrides limit their ability to cycle hydrogen reversibly at low temperature. For example, although LiBH4 is thermodynamically quite stable, the formation of LiBH4 from LiH + B requires elevated temperatures and pressures of up to 600 C and 150 bar. Here, we report ternary borides with active boron species that can be hydrogenated forming [BH4]1− anions at temperatures as low as ~280 C. These ternary borohydrides were prepared through milling of precursors followed by thermal treatment under inert atmosphere. Samples were then milled with additional binary hydrides before hydrogenation. Analysis using FTIR and 11B MAS NMR indicated that the ternary borides were hydrogenated to [BH4]1− species with good kinetics. After hydrogenation, the mixture could be cycled with dehydrogenation occurring in two steps that begin at 280 C and 345 C, respectively. Characterization using FTIR, 11B MAS NMR, and XRD, indicates that the [BH4]1− anions are consumed in the first dehydrogenation step.

9:36AM Y24.00007 Thermodynamic and kinetic destabilization in LiBH4-based hydride systems, JOHN VAJO, WEN LI, PING LIU, HRL Laboratories, LLC — The LiBH4/MgH2 destabilized hydride system has attracted considerable attention recently because it is a reversible system, based on the [BH4]− anion, with a high hydrogen capacity (11.6 wt % gravimetric). However, hydrogen release during a temperature ramp occurs in two steps with dehydrogenation of MgH2 to Mg + H2 occurring first followed by reaction of Mg with LiBH4 to form LiH + MgB2 + H2. These two steps occur despite there being a direct reaction that is thermodynamically allowed at lower temperatures. In this talk we describe a LiBH4-based hydride system that is kinetically as well as thermodynamically destabilized. In this system, a direct (concerted) dehydrogenation reaction of LiBH4 occurs at temperatures lower than the dehydrogenation temperature of any of the components separately. In addition, the system is reversible with an equilibrium hydrogen pressure (based on preliminary measurements) that is ~20X higher than the pressure for the LiBH4/MgH2 system.

9:48AM Y24.00008 Structure and librational dynamics in borohydrides, MONIKA HARTL, Los Alamos National Laboratory, MICHAEL WOLVERTON, University of Arkansas - Little Rock, ALICE ACATRINEI, Los Alamos National Laboratory, ABHIJIT BHATTACHARYYA, University of Arkansas - Little Rock, LUKÉ DAEMEN, Los Alamos National Laboratory — Borohydrides are candidates for reversible hydrogen storage. The attention accorded to this class of materials is supported by extensive hydrogenation/dehydrogenation thermodynamic measurements. However, the understanding of the chemical reaction mechanisms remain uncertain. We used neutron diffraction and inelastic neutron scattering, together with a computational approach, to examine the connection between structure and dynamics in several borohydrides and the possible role played by dynamics in the approach to the underlying chemical reaction mechanisms. We used first-principles calculations to identify the defects that are relevant for H transport in MgH2 and NaMgH3. In both materials, the physically relevant defects are charged and diffusion is dominated by mobility of negatively charged interstitial H. Interestingly, the diffusion of these species occurs via concerted mechanisms with low energy barriers. To improve the charged interstitial H diffusivity, a series of transition-metal additives are screened to lower the formation energy of mobile defects. Our results provide a practical way to examine and alter H diffusion in light metal hydrides.

10:00AM Y24.00009 First-principles Study on the Vibrational Modes and Electronic Structure of Alkaline and Alkaline-earth Amides and Alanates, TAKAO TSUMURAYA, TATSUYA SHISHIDOU, TAMIO OGUCHI, Hiroshima University — Light alkaline and alkaline-earth metal hydrides such as amides M(NH2)2 and alanates M(AH)4, (M=K, Na, Li, Ca, and Mg) have attracted a growing interest as reversible hydrogen storage materials recently because of their innately high hydrogen contents. [1, 2] We study the electronic structure of the amides and alanates with different cations, focusing on the role of cation states from first-principles calculations based on the all-electron FLAPW method. Calculated breathing stretch vibration modes for these compounds are compared with measured infrared and Raman spectra. In the amides, we find a significant tendency such that the breathing stretch vibration frequencies and the structural parameters of NH22− may vary in accordance with the ionization energy of cation, which may be explained by the strength in hybridization between cation orbitals and molecular orbitals of (NH2)2−. We elucidate the microscopic mechanism of correlations between the breathing stretch vibration frequencies of N-H and structural parameters by analyzing the calculated electronic structure from a view point of the molecular-orbitals. A similar tendency in the alanates is also discussed. [1] P. Chen, Z. Xiong, J. Luo, J. Lin and K.L. Tan, Nature 420, 302 (2002). [2] B. Bogdanovi and M. Schwickardi, J. Alloys Compd. 253-254, 1 (1997).
10:12AM Y24.00010 Neutron spectroscopy of $\gamma$-AlH$_3$. ALEXANDER KOLESNIKOV, Oak Ridge National Laboratory, Oak Ridge, TN 37831, JASON GRAETZ, Brookhaven National Laboratory, Upton, NY 11973, CRAIG JENSEN, WALKER LANGLEY, University of Hawaii, Honolulu, HI 96822, VLADIMIR ANTONOV, Inst. Solid State Physics, RAS, Chernogolovka, Russia — The density of vibrational states, G(E), for $\gamma$-AlH$_3$ is measured by inelastic neutron scattering. The obtained spectrum noticeably differs from that of $\alpha$-AlH$_3$, because $\alpha$-AlH$_3$ has a structure built of corner-sharing AlH$_6$ octahedra, while the $\gamma$-AlH$_3$ is composed of both corner- and edge-sharing AlH$_6$ octahedra. The first acoustic phonon peak in the G(E) of $\gamma$-AlH$_3$ appears at a lower energy and the band of translational modes extends to higher energies (55 vs. 42 meV) than in the spectrum of $\alpha$-AlH$_3$. The bands of Al-H bending modes are observed at about the same energies of 60–140 meV in $\gamma$-AlH$_3$ and $\alpha$-AlH$_3$, only the structures of the bands are different. The Al-H stretching modes in the $\gamma$-phase show eight peaks in the range 145 to 265 meV, while in the $\alpha$-phase they exhibit only two peaks at 200 and 235 meV. The G(E) spectrum of $\gamma$-AlH$_3$ is in good agreement with recent simulations [Y. Wang et al., Phys. Rev. B 77 (2008) 014101], which took into account the existence of a unique double-bridge bond between certain Al and H atoms.

10:24AM Y24.00011 Cubic Metallic Phase of Aluminum Hydride Showing Improved Hydrogen Desorption. RALPH H. SCHEICHER, DUCK YOUNG KIM, Condensed Matter Theory Group, Department of Physics and Materials Science, Uppsala University, Uppsala, Sweden, RAJEEV AHUJA, CMT Group, Uppsala Univ.; Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden — AlH$_3$ is of great interest for hydrogen storage applications, with a particularly attractive feature being its large hydrogen capacity of 10 wt.%. Here we report the results of our density functional theory study of the dehydrogenation properties in a cubic phase of AlH$_3$. The metallic nature of the electronic structure entails a more favorable hydrogen removal energy which is lowered by 75% compared to the insulating hexagonal phase. This remarkable reduction in the Al-H bond strength might bear important consequences for feasible reductions of AlH$_3$ as an on-board hydrogen storage material for mobile applications. Suggestions are made how the cubic phase could be prepared and stabilized at ambient pressure by off-board quenching. See also: R. H. Scheicher, D. Y. Kim, S. Lebègue, B. Arnaud, M. Alouani, and R. Ahuja, Appl. Phys. Lett. 92, 201903 (2008) and D. Y. Kim, R. H. Scheicher, and R. Ahuja, Phys. Rev. B 78, 100102(R) (2008).

10:36AM Y24.00012 Regeneration of Aluminum Hydride studied with Raman Microscopy. DAVID LACINA, JASON GRAETZ, J.J. REILLY, Brookhaven National Laboratory — We are interested in developing new methods to form aluminum hydride directly from aluminum powder and hydrogen. Due to the low free energy of formation, aluminum and hydrogen require extremely high pressures to react and form the hydride. It is possible to form alone directly at low pressure when it is catalyzed with a small amount of titanium (2 mol %) and stabilized as an adduct. We have studied the formation of amine-alanes by direct hydrogenation of aluminum and have attempted to understand the mechanisms behind these reversible reactions and the role of the catalyst. We will present the results from our recent survey of possible reactions between aluminum, hydrogen and various amines. We will also present the results of a Raman spectroscopy study of the alane polymorphs at ambient and high pressure and alane amines.

Friday, March 20, 2009 8:00AM - 11:00AM – Session Y25 DMP: Focus Session: Graphene XVIII: Functionalization and Growth II 327

8:00AM Y25.00001 Edge states and nitrogen substitutional doping in carbon nanoribbons. JIE JIANG, NC State U., Raleigh, WENCHANG LU, JERRY BERNHOLC, NC State U., Raleigh; CSMD, ORNL; PIOTR BOGUSLAWSKI, NC State U., Raleigh; IPPAS, Poland — The edge states in carbon nanoribbons and the electronic and magnetic properties in N-doped carbon nanoribbons are investigated within density functional theory. While the ground state of zigzag nanoribbons is spin polarized, defects lead to the spin carrier to be delocalized into the armchair edge, which results in a non-magnetic ground state. Scanning tunneling microscopy will thus show different features depending on edge quality. Turning to substitutionally doped carbon nanoribbons, the impurity states are elongated along the ribbon width by edge and confinement effects, which also affect their ionization energies in armchair ribbons. Formation energy calculations reveal that N atoms preferentially occupy edge sites in carbon nanoribbons. The extra electron from the donor suppresses the spin-polarization and tailors the relative magnetization at the two edges in zigzag ribbons. The interplay of impurity and edge states in zigzag ribbons leads to rich electronic effects, resulting in semiconducting or metallic behavior depending on the dopant position.

8:12AM Y25.00002 Counting Graphene Layers on Glass by Optical Reflection Microscopy. HELGI SKULASON, PETER GASKELL, CHRIS RODENCUK, THOMAS SZKOPEK, McGill University — Using optical reflection microscopy we can locate and count graphene layers on a bulk glass substrate. This is a reliable and low cost technique for graphene flake metrology. Optical reflection measurements are in agreement with the universal optical conductance of graphene. We present measurements of the optical conductivity of graphitic flakes showing a transition from few layer graphene to bulk graphite.

8:24AM Y25.00003 Molecular Physisorption on Graphene. DAVID CAREY, THOMAS CONNOLLY, University of Surrey — Ab initio calculations using both LDA and GGA functionals have been used to examine the binding energy, optimum binding intermolecular separations, molecular orientation dependence for a range of graphene lattice sites with oxygen containing molecules such as CO and NO. For all sites investigated NO has a higher binding energy than CO. For example, we find that the most stable sites are for the intermolecular axis parallel to the plane of the graphene layer with a binding energy of 195 meV for NO and 131 meV for CO using LDA VWN functional. Using the GGA PW91 functional the corresponding binding energies are 45 meV and 28 meV. When the CO or NO molecular axis is perpendicular to the graphene layer, orientation with the O atom oriented away from the graphene layer has a higher binding energy than CO. For example, we find that the most stable sites are for the intermolecular axis parallel to the plane of the graphene layer with a binding energy of 195 meV for NO and 131 meV for CO using LDA VWN functional. Using the GGA PW91 functional the corresponding binding energies are 45 meV and 28 meV. When the CO or NO molecular axis is perpendicular to the graphene layer, orientation with the O atom oriented away from the graphene layer is favored to be favored than those with the O atom closer to the graphene layer. Molecular physisorption on graphene is discussed.

8:36AM Y25.00004 Interface structure for growth of epitaxial graphene on SiC(0001). S.H. RHIM, G. SUN, L. LI, M. WEINERT, U. Wisconsin-Milwaukee — In spite of the enormous effort devoted to the study of the epitaxial growth of graphene on SiC, there is not yet a consensus regarding the structure of the interface between graphene and the substrate. There have been a long standing discrepancy between low energy electron diffraction (LEED) and STM patterns regarding the periodicity of graphene on SiC(0001); the theoretical studies of the of $6\sqrt{3} \times 6\sqrt{3}$ or $\sqrt{3} \times \sqrt{3}$ periodicity, while describing some aspects, disagree in important details with scanning tunneling microscopy (STM) images. We present a combined theoretical and experimental study, employing density functional calculations and STM, to investigate this issue. We propose the formation of a defected graphene layer at the interface, and then subsequent growth of graphene. The calculated bias-dependent STM images are in good agreement with our STM images, and provide insight into the details of the interface structure.

1Supported by DOE (DE-FG02-05ER46228) and NSF (DMR-0706359)
8:48AM Y25.00005 In-situ IR studies of graphene oxide reduction.  
\footnote{Work supported by the Southwest Academy for Nanoelectronics funded by SRC-NRI.}

MUGE ACIK, LAURENCE GOUX, YVES CHABAL — Thermal reduction of graphene oxide \( (GO) \) synthesized by Hummer’s method is studied by in-situ infrared absorption spectroscopy in a vacuum reactor. Initially, water and hydroxyl groups are removed \( (100^\circ \text{C}) \), with release of \( \text{CO}_2 \). Upon reduction of epoxides and carbonyl groups, the appearance of sp2-bonded carbon \( (C=C) \) bonds is evident with detection of in-plane and out of plane vibrations. However, oxygen remains in the structure in the form of COC bonds even after \( 700^\circ \text{C} \) anneal. Around \( 290^\circ \text{C} \), a strong increase of the absorbance associated with structure changes of \( GO \) is observed. The increase of the refractive index is attributed to an increase of electrical conductivity after reduction of \( GO \).

9:00AM Y25.00006 AFM local oxidation nanolithography of graphene

LISHAN WENG, LIYUAN ZHANG, YONG P. CHEN, LEONID P. ROKHINSON, Purdue University — We demonstrate the local oxidation nanopatterning of graphene films by an atomic force microscope. The technique provides a method to form insulating trenches in graphene flakes and to fabricate nanodevices with sub-nanometer precision. By utilizing this technique, a nanowide nanoribbon and submicron size nanoring were fabricated from a graphene flake. In addition we found that either trenches or bumps can be written on the graphene surface depending on the lithography conditions. It is proposed that the trenches are created by defect-associated oxidation whereas the bumps are incorporation of oxygen into the graphene lattice. Some of the bumps disappear with time as quickly as in a few minutes or as slow as in a few days. We also further investigate the possibility to remove the bumps in a controllable manner by writing trenches on top, applying opposite voltage or change the environmental conditions.

9:12AM Y25.00007 Hydrogen Saturation of Graphene Nanoribbons: edge states suppression and gap behavior

THIAGO MARTINS, ANTONIO J. R. DA SILVA, ADALBERTO FAZZIO, Physics Institute - University of Sao Paulo — Di-hydrogenated zigzag edges Graphene Nanoribbons \( (2H-ZZ-GNR) \) are more stable than the usually studied mono-hydrogenated \([1]\) passivation \( (H-ZZ-GNR) \). Using density functional theory, we studied a variety of \( H-ZZ-GNR \) configurations. We investigated how the interaction between the \( CH_2 \) units depends on their separation at the same edge as well as on the width of the ribbon. We observe, in agreement with previous studies \([1]\), that the \( 2H-ZZ-GNR \) passivation suppresses the presence of edge states, thus eliminating the magnetic instability of \( H-ZZ-GNR \) that is responsible for the gap opening in the anti-ferromagnetic ground state configuration. Moreover, there is a reduction of coupling between edge and bulk carbon atoms, resulting in a band structure whose gap is dominated by bulk bands and confinement effects. We also studied the behavior of the gap as a function of the ribbon’s width, and we observed that it quickly closes as the width is increased.


9:24AM Y25.00008 Anomalous magnetic susceptibility and Hall effect from valley degrees of freedom

TIANYI CAI, WANG YAO, The university of Texas at Austin, JUNREN SHI, Chinese Academy of Science, QIAN NIU, The university of Texas at Austin — With a staggered sublattice potential, sizable gaps can occur in epitaxial graphenen films. Magnetic and transport properties of this system are studied. We predict large signal of magnetic susceptibility and relate it to the intrinsic large magnetic moments of electrons. There is also an anomalous contribution to the ordinary Hall effect, which is due to the valley dependent Berry phase.

9:36AM Y25.00009 ABSTRACT WITHDRAWN

9:48AM Y25.00010 Si diffusion on and between graphene sheets

LEDE XIAN, M.Y. CHOU, School of Physics, Georgia Tech — The growth of epitaxial graphene \( (EG) \) on the SiC substrate is accompanied by the evaporation of Si atoms during the growth process. The continuing loss of Si atoms takes place even after the surface graphene sheets have been formed. This atomic transport is believed to be a key element in establishing a growth mechanism to model and control the process. Using density functional theory \( (DFT) \) calculations, we have studied the diffision of Si atoms on a single layer of graphene and between graphene sheets. The potential energy surfaces are explored. For single-layer graphene, the diffusion barrier for Si is relatively low. While for multilayers, some buckling of graphene sheets will appear and the stacking pattern also plays a role. The connection with the growth process will be discussed.

10:00AM Y25.00011 Gauge field for the edge states in graphene

KEN-ICHI SASAKI, Department of Quantum Matter, AdSM, Hiroshima University, Japan, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology and PRESTO, JST, Japan, RIICHIRO SAITO, Department of Physics, Tohoku University, Japan — By considering a continuous model for graphene, we study a special gauge field for the edge state. The gauge field explains the properties of the edge state such as the existence only on the zigzag edge, the partial appearance in the \( k \)-space, and the energy position around the Fermi energy. The gauge field polarizes the pseudospin. The applications of the gauge field to the ferromagnetism of edge states and the electron-photon interaction are reported on.

10:12AM Y25.00012 Collective properties of magnetobie excitons in quantum wells’ and graphene superlattices

OLEG BERMANN, ROMAN KEZERASHVILI, New York City College of Technology of CUNY, YURLII LOZOVIK, Institute of Spectroscopy — The Bose-Einstein condensation and superfluidity of quasi-two-dimensional spatially indirect magnetobie excitons in a slab of superlattice with alternating electron and hole layers consisting from the semiconducting quantum wells \( (QW) \) and graphene superlattice in high magnetic field are reported. The two different Hamiltonians of a dilute gas of magnetobie excitons with a dipole-dipole repulsion in superlattices consisting of both QWs and graphene layers \( (GL) \) in the limit of high magnetic field have been reduced to one effective Hamiltonian a dilute gas of two-dimensional excitons with the renormalized effective mass of the magnetobie exciton, which depends on the magnetic field. The instability of the ground state of the system of interacting two-dimensional indirect magnetobie excitons in a slab of superlattice with alternating electron and hole layers in high magnetic field is found. The stable system of indirect quasi-two-dimensional magnetobie excitons, consisting of pair of indirect excitons with opposite dipole moments is considered. The density of the superfuid component \( n_s(T) \) and the temperature of the Kosterlitz-Thouless phase transition to the superfluid state in the system of two- dimensional indirect magnetobie excitons, interacting as electrical quadrupoles, are obtained for both the QW and graphene realizations.

10:24AM Y25.00013 The Electronic Structure of Few-Layer Graphene: Probing the Evolution from a 2-Dimensional Sheet to a 3-Dimensional Solid by Optical Spectroscopy

KIN FAI MAK, MATTHEW SFEIR, JAMES MISIEWICH, TONY HEINZ, COLUMBIA UNIVERSITY, NEW YORK, NY 10027 COLLABORATION, BROOKHAVEN NATIONAL LABORATORY, UPTON, NY 11973 COLLABORATION — The evolution of the electronic structure of few-layer graphene, for \( n = 1, \ 2, \ 3, \ \ldots, \ 8 \) atomic layers, was characterized by optical absorption spectroscopy. Each thickness of few-layer graphene exhibited well defined and distinct infrared absorption peaks associated with interband transitions. The positions of the peaks were found to obey a simple scaling relation with layer thickness. The principal features of the experimental spectra for all samples could be described consistently in terms of the electronic states of the parent graphite material through application of a specific zone-folding construct obtained when only nearest-layer interactions are considered. Both the experiment and analysis permit one to follow the convergence of the multilayer graphene response to that of graphene with increasing sample thickness.
10:36 AM  Y25.00014  Edge effects in Bilayer Graphene Nanoribbons1, MATHEUS P. LIMA, ADALBERTO FAZZIO, ANTONIO J. R. DA SILVA, Physics Institute - University of Sao Paulo — We investigate the geometrical and electronic structure of zigzag bilayer graphene nanoribbons (B-ZGNR), with widths that range from \( w = 0.6 \) to \( w = 4.5 \) nm. The layers are in the Bernal stacking, which means that there are two types of C atoms, those that are positioned above the center of the hexagons of the other layer, defining a B-sublattice, and those right on top of the C atoms of the other layer, forming an A-sublattice. When we cut the layer along the zigzag edge, there are two possible alignments, \( \alpha \), where the outermost edge atoms belong to the A-sublattice, and \( \beta \), where the outermost edge atoms belong to the B-sublattice. Thus, only the inter-layer edge interaction differs. We found that the \( \alpha \) alignment is energetically favorable, with an inter-layer edges attraction, whereas for the \( \beta \) there is an inter-layer edges repulsion. These edge-related forces cause a deviation from the exact Bernal stacking, resulting in a non-monotonic behavior of the energy gap with the width \( w \) for the \( \beta \)-B-ZGNR, with a maximum value at \( w \approx 3.5 \) nm. This is a consequence of the competition between bulk and strongly attractive edge interactions. All results were obtained using density functional theory calculations with the inclusion of parameterized van der Waals interactions.

1We acknowledge financial support from FAPESP and CNPq.

10:48 AM Y25.00015  Measuring a Butterfly with Graphene, ANDRES CONCHA, Johns Hopkins University — The Hofstadter butterfly (HB) is a hierarchical structure that emerges as a consequence of the commensuration of two length scales, the magnetic length \( l \sim \frac{1}{\sqrt{B}} \) and the lattice spacing \( a \) between atomic sites. We argue that by using a set of scalar potentials and an external magnetic field it is possible to measure and manipulate the HB in graphene. Our claim is based in the fact that in graphene, close to the Dirac point the theory becomes critical and as such no length scale is present in the low energy description. Thus the only relevant length scales are dictated by the magnetic length and the distance between potential barriers. It is shown that the Hall conductance in the minigaps should be directly measurable with current available technology.

Friday, March 20, 2009 8:00AM - 11:00AM – Session Y26 DCMP: Glassy and Amorphous Systems 328

8:00AM Y26.00001  Long Term Aging of As<sub>x</sub>Se<sub>1-x</sub> glasses and the Intermediate Phase<sup>1</sup>, PING CHEN, JACOB WACHTMAN, P. BOOLCHAND, University of Cincinnati — The reversibility window in As<sub>x</sub>Se<sub>1-x</sub> glasses was reported<sup>2</sup> 8 years ago to reside in the 28% < \( x \) < 37% range. We have re-examined those samples in modulated DSC and Raman scattering. Both the 8 year old hermetically sealed samples in Al holders (set A) and samples from the same batch preparation but stored in plastic vials (set B) at laboratory ambient environment were studied. The reversibility window in samples of set A, after 8 years of aging, is found to be intact. In set B, analysis of the T<sub>g</sub> endotherm becomes difficult because of a precursor exotherm that appears in the 32% < \( x \) < 60% range, and steadily increases with \( x \). In addition, in both set of samples, one observes a sub T<sub>g</sub> endotherm upon aging in the 90 °C < T < 120 °C range. These m-DSC results supported by Raman scattering suggest that the exotherm is due to light induced nanocrystallization (nc) of As<sub>x</sub>Se<sub>y</sub> fragments (an extrinsic effect), while the sub-T<sub>g</sub> feature is due to nc fragments of trigonal Se formed upon long term aging (an intrinsic effect). These findings will be compared to a recent report<sup>3</sup>.

1Supported by NSF grant DMR 04-56472.

8:12AM Y26.00002  Molecular structure of virgin and T<sub>g</sub> cycled (Ag<sub>2</sub>Se)<sub>x</sub> (AsSe)<sub>1-x</sub> bulk glasses<sup>1</sup>, JACOB WACHTMAN, PING CHEN, P. BOOLCHAND, University of Cincinnati — AsSe, the base glass (x = 0) in the titled ternary, is an interesting example of a chalcogenide that is partially de-mixed into As<sub>2</sub>Se<sub>4</sub> molecules segregated from a connected AsSe network, with the latter determining glasses and the Intermediate Phase. Raman scattering reveals sharp modes of the Realgar molecules that are superimposed on broad modes coming from the backbone. Upon T<sub>g</sub> cycling virgin samples (as quenched melts), the concentration of de-mixed As<sub>2</sub>Se<sub>4</sub> molecules decreases, suggesting that thermally induced polymerization occurs; molecules break up to form part of the connective tissue. Modulated DSC experiments reveal a broad exotherm near 140 °C in virgin samples, which becomes nearly extinct in T<sub>g</sub> cycled samples. The exotherm may represent Realgar molecules nano-crystallizing as the temperature approaches T<sub>g</sub>. Compositional trends in thermal parameters such as T<sub>g</sub>, ∆C<sub>p</sub>(x), and the ∆H<sub>nr</sub>(x) as a function of Ag<sub>2</sub>Se content ‘x’ of the glasses will be reported.

1This work was supported by NSF Grant DMR 04-56472.

8:24AM Y26.00003  Atomic Picture of the Intermediate Phase in Ge<sub>x</sub>Sel-<x> glasses: A Joint Theoretical and Experimental Study<sup>1</sup>, FAKHAR UL INAM, GANG CHEN, Ohio University, DENYAGO TAFEN, West Virginia University, DAVID DRABOLD, Ohio University — Raman and calorimetric studies on GeSe1-x glasses have provided evidence for the existence of the intermediate phase (IP) in chalcogenide and other glasses. Here, Ab-initio molecular dynamics (MD) based models of these glasses are discussed, and an atomistic picture of the IP, based upon the models and available experiments, is presented. A thorough analysis of our models reveals that the IP in GeSe1-x glasses appears due to the competition between the percolating GeSe2 phase and the a-Se phase, which gives rise to the “flattening” of the observables in the IP window. We present X-Ray Absorption Near Edge Structure (XANES) measurements on germanium selenide glasses in the IP composition range, and detect an electronic signature of the IP in terms of the shift of the XANES white line (WL) and non-linear behavior of their intensities in the IP window. We show that these models appear to properly represent the XANES results.

1We wish to strongly acknowledge Prof. P. Boolchand for providing the samples we employed in the XANES work. Grants and Supports from NSF and U. S. Department of Energy is gratefully acknowledged.

8:36AM Y26.00004  Boson modes and Floppy modes in network glasses<sup>1</sup>, D. NOVITA, PING CHEN, P. BOOLCHAND, University of Cincinnati — Network glasses differ from their crystalline counterparts in a significant way— the presence of an excess of low-frequency vibrations. Here we show that in a covalent (As<sub>2</sub>S<sub>1-x</sub> and in a super-ion(1) (Ag<sub>x</sub>I<sub>1-x</sub>) glass system, Raman Bose peak scattering strength (I<sub>B</sub>) displays commonalities; in the flexible phase of these systems, I<sub>B</sub> is found to increase almost linearly as networks become more flexible or their connectivity decreases. Moreover, the rate at which dI<sub>B</sub>/dr changes is reminiscent of the variation dI<sub>f</sub>/dr of the floppy mode count (f) with r in rigidity theory. These results suggest that at least in the flexible phase, contributions to the boson peak must result in large part from floppy modes.

1This work was supported by NSF Grant DMR 04-56472.
2P. Chen et al. ArXiv 0810.3637.
8:48AM Y26.00005 Characterization of dry B$_2$O$_3$ glass$^1$, K. VIGNAROOBAN, D. NOVITA, PING CHEN, P. BOOLC-HAND, University of Cincinnati — A sample of Puratronic B$_2$O$_3$ (Aesar) was vacuum (10$^{-6}$ Torr) melted in a Pt crucible at 520°C for 3 days and slow cooled to room temperature to obtain a glass. All sample manipulations were performed in a N$_2$ gas purged glove box. $T_g$ of the sample from inflexion point of the reversing heat flow in an m-DSC experiment, using a scan rate of 3°C/min, gave a value of $T_g$ (mDSC) = 308(1)°C. A traditional DSC experiment, using a scan rate of 10°C/min, gave a value of $T_g$ (DSC) = 309(2)°C. Our $T_g$ (DSC) value is 12°C to 20°C higher than previous reports$^2$ using the same scan rate. Vibrational features in IR reflectance in the 1200-1600 cm$^{-1}$ range (LO and TO modes), and in the 3200-3600 cm$^{-1}$ range (free and bonded water) evolve as transparent platelets are exposed to laboratory environment, providing evidence for water reactivity of dry samples. Raman scattering results complement IR reflectance ones. We confirm$^2$ density of dry samples (1.805(4)gms/cm$^3$) to be somewhat less than wet ones (1.815(4) gms/cm$^3$).$^2$ Ramos et al. JNCS 221, 170 (1997).$^1$ F. Galeener et al, PRB 22, 3983 (1980).

3This work was supported by NSF Grant DMR 04- 56742.

9:00AM Y26.00006 Silicon under mechanical shear: molecular dynamics study, ALI KERRACHE, NORMAND MOUSSEAU, LAURENT J. LEWIS, Univ. of Montreal — Relaxation processes and defect behavior in amorphous silicon (a-Si) under shear are investigated by molecular dynamics simulations using the empirical Environment Dependent Inter-Atomic Potential. Shear deformations allow us to reproduce a vast range of interesting dynamics in disordered materials. For example, it has been shown recently that high-energy ion irradiation deforms plastically a-Si samples, following a pattern similar to the application of a shear. While large shear reproduce high-irradiation effects, moderate one can accelerate defect diffusion. A controlled application of shear can therefore help us to understand better the nature of defect diffusion in a-Si, in addition to generating new defects that could be placed with the appropriate external field at critical positions or even lead, in some cases, to crystallization of the a-Si. The properties of a-Si under shear are analyzed as a function of imposed shear velocity and as a function of the distance from the wall.

9:12AM Y26.00007 Liquid-liquid transition in supercooled silicon determined by first-principles simulation, P. GANESH, Geophysical Laboratory, Carnegie Institution of Washington, M. WIDOM, Department of Physics, Carnegie Mellon University — First principles molecular dynamics simulations reveal a liquid-liquid phase transition in supercooled elemental silicon. Two phases coexist below T$_c$ $\approx$ 1232K. The low density phase is nearly tetra-coordinated, with a pseudogap at the Fermi surface, while the high density phase is more highly coordinated and metallic in nature. The transition is observed through the formation of van der Waals loops in pressure-volume isotherms below T$_c$.

9:24AM Y26.00008 High thermal conductivity of a hydrogenated amorphous silicon film, J.L. FELDMAN, George Mason University, XIAO LIU, Naval Research Laboratory, D.G. CAHILL, University of Illinois, R.S. CRANDALL, National Renewable Energy Laboratory, NOAM BERNSTEIN, D.M. PHOTIADIS, M.I. MEHL, Naval Research Laboratory, D.A. PAPACONSTANTOPOULOS, George Mason University, HO-SOON YANG, Pusan National University, Korea — We measured the thermal conductivity $\kappa$ of an 80 nm thick hydrogenated amorphous silicon (a-Si:H) film from 80K to room temperature with the 3$\mu$m method and at room temperature with the time-domain thermoreflectance (TDTR) method. The a-Si:H sample with 1 at.% hydrogen was prepared by hot-wire chemical-vapor deposition (HWCDV), a procedure which was found previously to produce superior material properties with a near absent atomic tunneling states that are ubiquitous in glasses. We find that $\kappa$ is higher than any of the previous temperature dependent measurements, and shows a strong phonon mean free path dependence. We also performed numerical calculations on three 1000 atom models using Kubo theory and a tight binding electronic structure method. Due to the restrictions of the TDTR results on low frequency extrapolations of calculated phonon diffusivities, the Kubo thermal conductivity is seen to be too small to explain our experiments. We conclude that the HWCDV a-Si:H sample has superior structural ordering relative to any amorphous silicon previously studied.

9:36AM Y26.00009 Specific heat of amorphous materials outside of the universal regime: a-Si and a-Si:H, DANIEL QUEEN, University of California, Berkeley, QI WANG, RICHARD CRANDALL, National Renewable Energy Lab, FRANCES HELLMAN, University of California, Berkeley — We present specific heat measurements for a-Si and a-Si:H films that are known to lack the broad distribution of tunneling level systems (TLS) as measured by internal friction. Below 1K the TLS model describes the universal behavior seen in specific heat, thermal conductivity, and other measurements. However, this model does not address the universal high temperature features, namely, the plateau in $\kappa$ and peak in $\frac{C}{T}$ that occur around 10K. Tetrahedrally bonded systems, such as a-Si and a-Ge, have long been thought to lack TLS due to the over constrained nature of their bonding. These materials prove difficult to quench from a bulk melt but are routinely grown by vapor deposition. We use our MEMS nanocalorimeter for heat capacity measurements between 2-300K on a range of a-Si and a-Ge films prepared by e-beam evaporation and Hot-wire CVD. Changes in the high temperature specific heat will be discussed for films that are known to have orders of magnitude lower densities of TLS as measured by internal friction.

9:48AM Y26.00010 Hydrogen microstructure and voids in amorphous silicon hydride: A first principles study, RAJENDRA TIMILSINA, PARTHAPRATIM BISWAS, University of Southern Mississippi — We study distribution of hydrogen in amorphous silicon hydride configurations in several models of a-Si:H using first-principles density functional calculations. Motivated by recent experimental results via small angle $x$-ray scattering, which reveals the presence of large voids (of linear dimension up to 4 nm) in a-Si:H, we develop models for a range of concentration, and study the effect of voids on hydrogen distribution. In particular, we investigate the presence of voids in two different concentration regime: high (14 at. % and above) and low (below 14 at. %) following a recent experimental observation from infrared absorption spectroscopy. The bonding environment of H atoms, and the local electronic structure near the voids are also presented.

10:00AM Y26.00011 Atomistic modeling of amorphous silicon carbide: A first-principles study, PARTHAPRATIM BISWAS, University of Southern Mississippi, RAYMOND ATTA-FYNN, University of Texas, Arlington — Localized basis ab initio molecular dynamics techniques within density functional theoretic framework have been used to model a realistic atomistic configuration of amorphous silicon carbide (a-Si$_{1-x}$C$_x$)$_{3}$ containing 1000 atoms. The structural, electronic and vibrational properties have been studied and compared to existing theoretical models and available experimental data. Our study clearly reveals that the short-range chemical order in this material is predominant due to presence of heteronuclear Si-C bonds with coordination defect concentration less than 5% and the chemical disorder parameter was $\chi = 0.083$. Our 1000-atom model shows the presence of a clean gap in the spectrum and we also study the nature of the localization of the electronic band tail states as well as the vibrational eigenmodes.

1University of Southern Mississippi, Grant No. DE00945

10:12AM Y26.00012 ABSTRACT WITHDRAWN —
10:24AM Y26.00013 Glass Formability of Aqueous Solutions, and the Critical Nucleation Radius of Cubic Ice, Ryan Dunn, Matthew Warkentin, Robert Thorne, Cornell University — We have determined critical cooling rates and critical warming rates for a range of concentrations of different solutes in aqueous solutions using high-speed video microscopy. Our results show that the glass formability of aqueous solutions is exponential in the concentration for all solutes tested, with a different characteristic concentration for each solute. The characteristic concentration correlates with molecular radius. A simple modification of critical droplet theory relates the characteristic concentration to the critical nucleation radius in pure water, and explains the relationship between molecular radius and the characteristic. This simple, general theory of glass formability in aqueous solutions is important at a fundamental level, and will also have broad consequences for the field of cryobiology.

10:36AM Y26.00014 Nanocalorimetry as a means to explore thin films of vapor-deposited organic glasses, Kenneth L. Kearns, Department of Chemistry, University of Wisconsin-Madison, Heiko Huth, Mathias Ahrenberg, Christoph Schick, Institute of Physics, University of Rostock, M. D. Ediger, Department of Chemistry, University of Wisconsin-Madison — Vapor deposition was used to prepare nanometer thick films of small molecule organic glasses. Films of indomethacin (IMC) and 1,3,5-tris(naphthyl)benzene (TNB) with a range of stabilities and thicknesses were created and characterized using differential nanocalorimetry. The heat capacity-like calorimetric signal was lower for the stable vapor-deposited glass films at temperatures below the glass transition $T_g$ than for an ordinary glass prepared by cooling the liquid. A gradual increase in the calorimetric signal was observed during the isothermal transformation above $T_g$ from stable to ordinary glass with the fastest transformation taking place in about 200 $\tau_m$. The time for this transformation was dependent on film thickness with 350 nm thick films transforming approximately 5 times faster than 40 $\mu$m thick films. Aging experiments on the ordinary glass also showed a thickness dependence with thinner films aging more rapidly. This thickness dependent behavior is consistent with a mechanism where the dynamics at the film interfaces are faster than those in the bulk.

10:48AM Y26.00015 Evidence for a new molecular packing at low temperatures in vapor-deposited indomethacin, Kevin Dawson, Ken Kearns, Werner Steffen, Lian Yu, Mark Ediger — Thin films of the low molecular weight organic glass former indomethacin were prepared at different substrate temperatures using physical vapor deposition. When analyzed by wide angle x-ray scattering, samples prepared at $T_D$-50 K showed a broad high intensity peak that is not present in samples prepared at $T_D$. When such samples were annealed at $T_g$-4 K the extra peak eventually vanished but only after 24,000 s (more than 500 $\tau_m$). At low deposition rates the WAXS signature of this new molecular packing is only observed for substrate temperatures below $T_g$-20 K. Based on WAXS data on supercooled indomethacin, the new WAXS peak is unexpected. These results suggest that ordinary indomethacin glasses aged to equilibrium 20 K below the conventional $T_g$ would undergo a first order transition to a new amorphous phase.

Friday, March 20, 2009 8:00AM - 10:36AM
Session Y27 DCMP: Mechanical Properties of Nanomaterials

8:00AM Y27.00001 Carbon nanotube dispersed liquid crystal: A nano electromechanical system, Rajratan Basu, Germano Iannacchione, Worcester Polytechnic Institute — Electric field induced director orientation of a nematic liquid crystal (LC) + carbon nanotube (CNT) system reveals insights on switching behavior for this anisotropic composite. Once the field goes off, the LC+CNT system relaxes back to the original orientation through a mechanical rotation, revealing the intrinsic dynamics. LC molecules and CNTs cooperatively form local pseudonematic systems in the isotropic phase due to strong LC-CNT interactions. These field-responsive anisotropic domains do not relax back to the original orientation on switching of the field off, which could find potential applications in memory devices.

8:12AM Y27.00002 Strong “position squared” optical readout of a micromechanical oscillator, Jack Sankey, Andrew Jayich, Benjamin Zwickl, Cheng Yang, Jack Harris, Yale University — Optomechanical devices with a flexible Si membrane inside an optical cavity allow for very high optical finesse and high mechanical quality factor in a single device. They also provide fundamentally new functionality: the cavity detuning can have a quadratic dependence on the membrane position. This enables a measurement of “position squared” ($x^2$) and in principle a QND phonon number readout of the membrane. However, the readout achieved using a single cavity mode is not sensitive enough to observe quantum jumps between phonon Fock states. Here we demonstrate an $x^2$-sensitivity that is orders of magnitude stronger using two nearly-degenerate transverse cavity modes, and that we can tune this sensitivity somewhat by tilting the membrane. We derive a perturbative treatment that describes the interactions between the transverse optical modes and achieve good agreement with observation using realistic parameters. We also show that the $x^2$-coupling should be easily tunable over a wide range via nm-scale membrane displacements along the cavity axis.

8:24AM Y27.00003 In-situ Transduction of the In-Plane and Out-of-Plane Modes of Nanowire-based Very-High Frequency Electromechanical Resonators, Wayne Fung, Wei Lu, University of Michigan — Recent advances in nano-electromechanical systems (NEMS) promise important applications such as mass and force sensing, rf signal generation and timing, and quantum measurement studies. Chemically synthesized nanowires appear especially attractive for NEMS because of their atomically smooth surfaces and large aspect ratios. Here we report the measurements of doubly-clamped beam mechanical resonators using SnO$_2$ nanowires with widths ranging from 30 to 80 nm. The devices are electrostatically actuated and detected on-chip using a dual-gate setup and an all-electronic transduction scheme. This setup also allows us to independently actuate and tune the resonant frequencies of both the in-plane and out-of-plane modes of vibration in situ, potentially leading to NEMS-based practical applications. Our devices exhibit resonant frequencies ranging from 30 to 100 MHz, quality factors up to 2000, force sensitivities down to $10^{-14}$ N/Hz$^{1/2}$, and mass sensitivities down to $5 \times 10^{-17}$ g. The frequency of the in-plane and out-of-plane modes can be tuned within $\pm 1$ MHz of their nominal values at gate voltages of $\pm 5$ V.

8:36AM Y27.00004 ABSTRACT WITHDRAWN

8:48AM Y27.00005 Mechanical properties of metal-repaired defective carbon nanotubes, Guang-Ping Zheng, Hong Kong Polytechnic University, Kowloon, Hong Kong — Carbon nanotubes (CNTs) are promising in the production of strong and light structural materials because of their unique mechanical properties such as ultrahigh mechanical strength and large ultimate tensile strain. However, CNTs are not totally defect-free. Instead, several types of intrinsic defects exist, hence the mechanical strength and ductility of CNT can be significantly lower than those of an ideal one. In this study, 3D transition-metal atoms (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) or clusters are filled into the defective sites of single-walled (SW) CNT containing vacancy defects, resulting in stable repaired SWCN. The mechanical and electronic properties of the repaired SWCNs are investigated by spin-polarized density functional theory. The results indicate that the 3D transition-metal atoms acting as substitutional defects can substantially modify the electronic structure and magnetization of an un-deformed CNT. Compared with defective SWCN, the metal-repaired CNT shows significant enhancements in mechanical strength and ductility that are close to or even better than those of pristine CNTs. The underlying physics of these behaviors are analyzed by the structural transformation, electronic structures and spin and charge distributions during the tensile tests. Strong magneto-mechanical coupling effect is found to be responsible for the enhanced mechanical behaviors of metal-CNT hybrid structures.
Mechanics of Nanometric Water Wire

Manhee Lee, Baekman Sung, Bongsu Kim, Jongwoo Kim, Wonho Jhe, Seoul National University — Water has been one of the perfect Newtonian viscous liquids, which are exactly described by Navier-Stokes equation. However, it has been found that the effective shear viscosity of water confined between mica crystals at few nanometer thickness is very different from the one of 3-dimensional bulk water. While some researchers have measured very high viscoelasticity of the confined liquid [1], the other researchers reported the fluidic nature of water confined between mica surfaces at <3.5 nm interfacial separation like bulk-water viscosity [2]. These conflicting results concerning the mechanical properties of nanometric water have been continually reported for the past several years. None of them clearly clarified the mechanical properties of nanometric water, and the detailed behavior of the viscoelasticity within a tip-sample separation less than 1 nm has not been measured. Here, we investigate a nanometric water cluster formed between AFM tip and sample surface and present the nano-mechanical properties of it including viscoelasticity, dissipation energy, and phase transitions. [1] Y. Zhu and S. Granick, Phys. Rev. Lett. 87, 096104 (2001). [2] U. Raviv, P. Laurat, and J. Klein, Nature (London) 413, 51 (2001).

Torsional Stick-Slip Behavior in WS₂ Nanotubes

K.S. Nagapriya, Ohad Goldbart, Ifat Kaplan-Ashiri, Weizmann Institute of Science, Rehovot 76100, Israel, GOTTTHARD SEIFERT, Technische Universität Dresden, D-01062 Dresden, Germany, RESHEF TENNE, ERNESTO JOSÉVICH, Weizmann Institute of Science, Rehovot 76100, Israel — We experimentally observed atomic-scale torsional stick-slip behavior in individual nanotubes of tungsten disulfide (WS₂). When an external torque is applied to a WS₂ nanotube, all its walls initially stick and twist together, until a critical torsion angle, at which the outer wall slips and twists around the inner walls, further undergoes a series of stick-slip torque oscillations. This is contrary to what happens in a multi-wall carbon nanotube, where an external torque causes the outer wall to slip and twist smoothly around the inner walls. We present a theoretical model based on DFTB calculations, which explains the torsional stick-slip behavior of WS₂ nanotubes in terms of the competition between the effects of the in-plane shear stiffness of the WS₂ walls and the inter-wall friction arising from the atomic corrugation of the interaction between adjacent WS₂ walls. K. S. Nagapriya, Ohad Goldbart, Ifat Kaplan-Ashiri, Gotthard Seifert, Reshef Tenne, and Ernesto Joselevich, Phys. Rev. Lett. 101, 195501 (2008).

Optical Requirements for Quantum Mechanics with Micromechanical Systems

Dustin Kleckner, Brian Pepper, Physics Department, University of California, Santa Barbara, Evan Jeffrey, Petro Sonin, Huylens Laboratory, Universiteit Leiden, DIRK BOUWMEESTER, Physics Department, University of California, Santa Barbara and Huygens Laboratory, Universiteit Leiden — Interest in micro-optomechanical systems is motivated by the desire to test quantum mechanics on relatively massive scales. Proposals for realizing these effects have extremely challenging technical requirements, particularly with regards to optical quality. We present the results of simulations designed to determine the effects of imperfections in real systems on the maximum achievable optical finesse. Additionally, we will discuss recent progress in our efforts to fabricate novel devices with the required properties.

High-performance supercapacitors, actuators and elastomeric composites based on CNT assemblies

Mikhail Kozlov, Jiyoung Oh, Minkyoon Shin, Raquel Robles, Maricio Lima, Ray Baughman, University of Texas at Dallas — A number of materials ranging from carbon nanotube (CNT) yarns, sheets and CNT-based composites to shape memory alloys (SMA) have been explored for the application in the area of energy conversion and storage. Highly porous sheets comprised of Single Walled Carbon Nanotubes and doped poly-pyrrole (SWNT-PPy) were found to possess remarkably high specific capacitance of about 131 F/g. CNT-elastomeric polymer composites exhibited electrical conductivity of about 0.5 S/cm and can be stretched by 1400%. We found that if powered electrically, the isometric stress generation capability of commercial ferroelectrics and is significantly larger than that of natural muscles. We also report several types of artificial muscles that convert the chemical energy of high-energy-density fuels to mechanical energy. Because of more than 30 times higher energy density obtainable for fuels like methanol, compared to that for the most advanced batteries, the major expected benefits are dramatic increase in energy conversion efficiency, work capacity, power performance.

Determination of Intrinsic Damping in a MWNT using the Harmonic Detection of Resonance Method

Doyl DickeL, Gayatri Keskar, Malcolm Skove, Apparao Rao, Clemson University, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634 COLLABORATION, CENTER FOR OPTICAL MATERIALS SCIENCE AND ENGINEERING TECHNOLOGIES, CLEMSON UNIVERSITY COLLABORATION — Harmonic Detection of Resonance (HDR) method has been shown to be an effective method of electrically determining the resonant frequency of cantilevered structures at both the micro- and nanometer scale. Previously, HDR has been used effectively to study nonlinear behavior in highly anharmonic systems, as a gas sensor, and to determine the resonant frequency of a Macro scale Carbon Nanotube (MWNT). In addition, the HDR method has been used for determining the material properties such as the Young’s Modulus. Here, we provide a simple model describing the theory underlying the HDR method and a demonstration of its use in determine the resonant behavior of a MWNT. Finally, we report the effects of varying pressures on both the resonant frequency and quality factor of the MWNT. We also estimate the intrinsic damping inherent in the MWNT from these effects and show its correlation with defect density. The MWNT examined was found to have a resonant frequency for its primary mode of oscillation of 2.79 MHz with a quality factor of 10.15 at a pressure less than 1 Pa.

Eigenmodes and Vibration Spectra of Ag₂Ga Nanoneedles Measured Using Laser Doppler Vibrometry

R. Reifenberger, L. Biedermann, T. Tung, A. Ramam, Birck Nanotechnology Center, Purdue University, M. Yanzdanpanah, ElectroOptics Research Institute and Nanotechnology Center, U. of Louisville and Naugatucelles LLC, R. Cohn, ElectroOptics Research Institute and Nanotechnology Center, U. of Louisville — Applications for selectively grown Ag₂Ga nanoneedles include high-aspect ratio conductive AFM tips, mass sensors, force sensors, and high resonant frequency nano-cantilevers. To help enable these applications, reliable estimates for the elastic modulus of these nanoneedles and the quality factors of their oscillations are of interest. We have used Laser Doppler Vibrometry (LDV) to measure the vibration spectra and eigenmodes of individual Ag₂Ga nanoneedles. An advantage of this technique is that the vibration spectra between 0 and 20 MHz can be measured with high frequency resolution, allowing the eigenfrequencies and quality factors of each resonance to be accurately determined. Using Euler-Bernoulli beam theory, the elastic modulus and spring constant can be calculated from the nanoneedles’ eigenfrequencies and the dimensions of the nanoneedles. The techniques developed can be used to measure the vibrational spectra of any suspended nanowire with high frequency resolution.
10:24AM Y27.00013 Digital Batteries1, ALFRED HUBLER, University of Illinois at Urbana-Champaign — The energy density in conventional capacitors is limited by sparking. We present nano-capacitor arrays, where - like in laser diodes and quantum wells [1] - quantization prevents dielectric breakdown. We show that the energy density and the power/weight ratio are very high, possibly larger than in hydrogen [2]. Digital batteries are a potential clean energy source for cars, laptops, and mobile devices. The technology is related to flash drives. However, because of the high energy density, safety is a concern. Digital batteries can be easily and safely charged and discharged. In the discharged state they pose no danger. Even if a charged digital battery were to explode, it would produce no radioactive waste, no long-term radiation, and probably could be designed to produce no noxious chemicals. We discuss methodologies to prevent shorts and other measures to make digital batteries safe. [1] H. Higurashki, A. Toriumi, F. Yamaguchi, K. Kawamura, A. Hubler, Correlation Tunnel Device, U. S. Patent No. 5,679,961 (1997) [2] Alfred Hubler, http://server10.how-why.com/blog/

Friday, March 20, 2009 8:00AM - 11:00AM – Session Y28 FIAP: Nanotechnology I 330

8:00AM Y28.00001 Nanoscale Assembly of Actuating Cilia-Mimetic1, LANCE BAIRD, JENNIFER BREIDENICH, BRUCE LAND, ALLEN HAYES, JASON BENKOSKI, Johns Hopkins University Applied Physics Laboratory, PEI KENG, JEFFREY PYLUN, University of Arizona — The cilium is among the smallest mechanical actuators found in nature. We have taken inspiration from this design to create magnetic nanochains, measuring approximately 1-5 µm long and 25 nm in diameter. Fabricated from the self-assembly of cobalt nanoparticles, these flexible filaments actuate in an oscillating magnetic field. The cobalt nanoparticles were functionalized with a polystyrene/benzaldehyde surface coating, thus allowing the particles to form imine bonds with one another in the presence of a diamine terminated polyethylene glycol. These imine bonds effectively cross-linked the particles and held the nanochains together in the absence of a magnetic field. Using design of experiments (DOE) to efficiently screen the effects of cobalt nanoparticle concentration, crosslinker concentration, and surface chemistry, we determined that the morphology of the final structures could be explained primarily by physical interactions (i.e. magnetic forces) rather than chemistry.

1 Johns Hopkins University Applied Physics Laboratory Internal Research and Development

8:12AM Y28.00002 Amplification by 1/f noise with stochastic resonance in silicon-based nanomechanical resonators. , DIEGO N. GUERRA, TYLER DUNN, PRITIRAJ MOHANTY, Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, MA 02215 — We report signal amplification by 1/f noise with stochastic resonance in a nanomechanical two-state system of a nonlinear silicon resonator. The addition of 1/f noise to a sub-threshold modulation signal enhances the likelihood of an electrostatically driven resonator switching between its two states in the hysteretic region. Considering the prevalence of 1/f noise in integrated circuits, signal enhancement demonstrated here, using a fully on-chip electronic actuation/detection scheme, suggests potentially beneficial use of the otherwise detrimental noise.

8:24AM Y28.00003 High Frequency Antennas for Wireless Transmissions of Audio and Video Signals Using Threads Spun From Long Multi-Wall Carbon Nanotubes. , DAVID MAST, CHAMINDA JAYASINGHE, MARK SCHULZ, VESSELIN SHANOV, University of Cincinnati — We have used threads spun from long multiwall carbon nanotubes (MWCNT) to make antennas for audio and video broadcasts (transmission and reception) at GHz frequencies. The MWCNT used to make the threads have outer diameters from about 6 nm to 30 nm. These MWCNT’s have been grown in lengths up to 18 mm. The diameter of the CNT threads used to fabricate the high frequency antennas was 25 microns. Initial measurements consist of 1) transmission and reception of a CW signals at f = 694 MHz and 1386MHz , 2) the transmission and detection of a CW signal plus sidebands at ± 100kHz, 3) the broadcast and reception of an AM modulated audio signal, 4) the broadcast and reception of composite video images, 5) the simultaneous broadcast and reception of audio signals from a single CNT antenna, and 6) the simultaneous transmission and/or reception at multiple frequencies from a single CNT thread antenna. The results of using the CNT thread antenna for these transmissions will be discussed.

8:36AM Y28.00004 Noise color and asymmetry in stochastic resonance with silicon nanomechanical resonators. , TYLER DUNN, DIEGO N. GUERRA, PRITIRAJ MOHANTY, Boston University Physics — Stochastic resonance (SR) with white noise has been well established as a potential signal amplification mechanism in nanomechanical two-state systems. While white noise represents the archetypal stimulus for SR, typical operating environments for nanomechanical devices often contain different classes of noise, particularly colored noise with a 1/f spectrum. As a result, improved understanding of the effects of noise color is necessary in maximizing device performance. Here, we report measurements of SR in a silicon nanomechanical resonator using 1/f noise and exponentially correlated Ornstein-Uhlenbeck noise. Power spectral densities and residence time distributions provide insight into asymmetry of the bistable amplitude states, and evidence suggests that 1/fα spectra with increasing noise exponent α may lead to increasing asymmetry in the system, reducing the achievable signal-to-noise ratio. Furthermore, we explore the effects of correlation time τ on SR with the use of exponentially correlated noise. We find monotonic suppression of the spectral amplification as the correlation time increases.

8:48AM Y28.00005 Room-Temperature Single-Electron Transistors fabricated using CMOS-compatible processes , VISHVA RAY, RAMKUMAR SUBRAMANIAN, PRADEEP BHADRACHALAM, SEONG JIN KOH, The University of Texas at Arlington — A critical requirement for the fabrication of single-electron devices is that the device components (Coulomb island, source, drain, and gate electrodes) be arranged with nanometer scale precision. We present a new single-electron device structure which consists of vertically stacked source and drain electrodes separated by a thin dielectric film. Using this configuration, we were able to control the gap between the electrodes with nanometer scale precision over an entire wafer, thereby allowing the concurrent fabrication of many device units in parallel processing. Coulomb islands (10 nm Au nanoparticles) were positioned in the gap between the source and the drain electrodes. Individually addressable gate electrodes were then incorporated in these devices, also in complete parallel processing. These devices have yielded clear single-electron transport characteristics (Coulomb blockade/staircase and Coulomb oscillations) at room temperature as well as at low temperatures (~10 K). The experimental data is in excellent agreement with the orthodox theory of single-electron tunneling. This study suggests that the fabrication of chip-level integrated systems of single-electron devices may now be possible using current CMOS fabrication technology. (ONR (N00014-05-1-0030), NSF CAREER (ECS-0449958), and THECB ARP (003656-0014-2006)).

1Supported by NSF Grant DMS 03-25039 ITR.
9:00AM Y28.00006 Electronic-structure modulation transistor: A new switch with few kT supply voltage, HASSAN RAZA, School of Electrical and Computer Engineering, Cornell University, Ithaca NY, 14853, TEHSEEN RAZA, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, TUO-HUNG HOU, Department of Electrical Engineering, National Chiao Tung University, Hsinchu, Taiwan 300, ROC., EDWIN KAN, School of Electrical and Computer Engineering, Cornell University, Ithaca NY, 14853. — We present a novel electronic-structure modulation transistor (EMT) for post-CMOS logic applications. The device is based on the electronic structure modulation of the channel by an external gate voltage. Its functionality is theoretically analyzed using single-band tight-binding model and non-equilibrium Green’s function formalism. We report that the EMT is expected to have very large ON/OFF current ratio with reasonable self gain using a few kT Vdd. We provide an experimental proof-of-concept device of the proposed mechanism in a double gated structure using a 20 nm long and 10 um wide channel consisting of Au nanocrystals (NCs) and nitride. Putting negative charge on the NCs is results in wavefunction extension over larger distance due to lifting of the energy levels, resulting in reduction of the effective barrier. In transfer characteristics, we find a non-linear dependence of the drain current on gate voltage and charge stored in the channel, which we attribute to the wavefunction modulation of the Au NCs due to charging.

9:12AM Y28.00007 The electronic structure of diodes probed under bias, PER-ANDERS GLANS, JINGHUA GUO. Advanced Light Source, Lawrence Berkeley National Laboratory, JEONG PARK, SOMORJAI GABOR, Materials Sciences Division, Lawrence Berkeley National Laboratory. — Chemists have known for decades that when metal nano-particles are affixed to a catalytically inactive oxide surface, the catalytic turnover rate of the array is more than 10 times that of a metal surface alone. However, the mechanism behind the effect is not clear. To understand the catalytic activity of the interface between the metal nano-structures and the oxide substrate, we have investigated the electronic structure of Pt and Pd doped diodes on a TiO2 substrate. The devices were put under bias during the measurements in an attempt to reproduce the potential differences found over the diode when used as a catalyst. This is challenging for electron based measuring techniques, but using photon-in, photon-out techniques we have successfully probed the electronic structure of Pt and Pd doped diodes under bias. The results from soft x-ray absorption and emission will be presented.

9:24AM Y28.00008 Spatial Wavefunction Switched Field-Effect Transistors (SWS-FETs): A Novel Device with Multiple States and Functionality, FAQUIR JAIN, EVAN HELLER, University of Connecticut. — An asymmetric coupled quantum well transport channel FET is shown to confine carriers in either the lower of the two wells, both wells, or upper well (adjacent to the gate insulator) depending on the gate voltage. That is, as the gate voltage is increased above threshold in n-channel FET, the electron wavefunction is spatially switched, which in turn change the operating characteristics. A Spatial Wavefunction Switched (SWS) FET, having two coupled wells in the channel, provides four states 00, 01, 10, 11 corresponding to wavefunction location. No wavefunction being the OFF (00 state), electrons in well W2 (01 state), in well W1 (10 state), and both Wells W1-W2 (11 state). Simulation has verified the spatial switching in SiGe as well as InGaAs coupled well FET structures. The wavefunctions/carrier locations get more pronounced and result in additional states when the transport channel is configured as a quantum dot (QD) channel. Preliminary simulation of quantum dot gate 3-state structures, configured as SWS-QD channel FET, will also be presented.

9:36AM Y28.00009 Ultrathin germanium-on-insulator tunneling field effect transistors, D. KAZAZIS, P. JANNTAY, A. ZASLAVSKY. Brown University, Div. of Engineering, Providence, RI 02912, C. LE ROYER, C. TABONE, L. CLAVELIER, CEA-LETI, Grenoble, France. — As the CMOS downscaling is approaching its limits, there is greater need for alternative and unconventional devices to continue enhancing the performance of electronics. We report on the fabrication and electrical characterization of a CMOS-compatible germanium-on-insulator (GeOI) tunneling field effect transistor (TFET) device that can in principle switch more sharply than a standard FET. The source-drain current in the TFET is based on interband tunneling between an inversion channel and a counterdoped drain electrode. Taking advantage of the narrower bandgap of germanium, the devices are fabricated in ultra-thin GeOI and consist of a heavily p-type doped, epitaxially grown drain, an n-type ion-implanted source and a standard high-k dielectric gate stack with channel lengths down to 400 nm. The devices exhibit a reasonable on-off current ratio of more than 10² and improved on current compared to silicon-on-insulator TFETs. Current-voltage measurements at room and low temperatures will be presented to characterize the behavior of the fabricated transistors.

9:48AM Y28.00010 Full Recovery of PFET NBTI and NFET PBTI of high-k metal gate MOSFETs with high temperature bake, ANASTASIOS KATSETOS, JAMES STATHIS, FERNANDO GUARIN. — High-k metal gate MOSFETs exhibit Bias Temperature Instability (BTI) degradation mechanisms. The p-channel Field Effect Transistor (PFET) has NBTI which results in threshold voltage (Vt) decrease and drive current (Ion) decrease when the gate is biased negatively with respect to the channel. The n-channel Field Effect Transistor (NFET) has PBTI which results in threshold voltage (Vt) increase and drive current (Ion) decrease when the gate is biased positively with respect to the channel. The amount of NBTI and PBTI is process dependent and depends on temperature, gate voltage, time and gate oxide thickness. PBTI has stronger dependence on voltage than NBTI and NBTI has stronger temperature dependence than PBTI. However, with a high temperature (370°C) bake, full recovery of both NBTI and PBTI is achieved and the devices behave like unstressed devices on repeated BTI stress.

1IBM Systems and Technology Group, S/C R&D Center, 2070 Rt 52, Hopewell Junction, NY 12533.
2IBM T.J. Watson Research Center Yorktown Heights, NY 10598.

10:00AM Y28.00011 Band Structure Engineering of PtSi, ALEX SLEPKO, ALEXANDER A. DEMKOV. The University of Texas — PtSi is being considered as a contact material in field effect transistors. It has an additional advantage of having a low Shottky barrier to p-type Si. The relatively low conductivity of PtSi compared for example to pure Pt can be traced to the low density of states at the Fermi level. In this theoretical study we discuss a method to increase the conductivity of PtSi by manipulating the density of states through alloying. The scheme is based on substituting Pt atoms by Ti atoms to shift the Fermi level to a higher density of states region. We find identify a compound with the carrier concentration 2.7 times larger than that of bulk PtSi. We estimate the formation energies of the compounds and determine the solubility limit of Ti in PtSi at room temperature. We analyze the effect of doping with Ti on the work function for the (121) surface (the lowest energy surface orientation of PtSi). Moreover, we study possible schemes to lower the formation energies of the alloys by further doping with boron, carbon, gallium and aluminum. We identify a stable alloy in the case of aluminum doping. All calculations are done within the framework of density functional theory.

1Supported by the Semiconductor Research Corporation under contract 2006-JV-1439.
10:12AM Y28.00012 Ideal SiC Schottky Barrier Diodes Fabricated Using Refractory Metal Borides\textsuperscript{1}. TOM ODER, RANI KUMMARI, Youngstown State University — We present results of n-type 4H-SiC Schottky barrier diodes fabricated using several refractory metal boride Schottky contacts deposited on SiC held at various temperatures. From the electrical properties determined by current-voltage measurements, diodes with contacts deposited on SiC substrates held at 600 °C had average ideality factors in the range 1.04 – 1.09 and Schottky barrier heights of 1.02 eV – 1.14 eV; and these values remained unchanged after the diodes were annealed at 600 °C for 20 min. Diodes with contacts deposited on substrates held at 20 °C had much higher ideality factors which decreased only slightly after the annealing. The Rutherford backscattering spectroscopy spectra of these contacts revealed a systematic decrease in oxygen with increase in the deposition temperature. The improved electrical properties and thermal stability are attributed to the removal of oxygen from the boride/SiC interface during high temperature deposition.

\textsuperscript{1}This research was supported by funds from the National Science Foundation

10:24AM Y28.00013 ABSTRACT WITHDRAWN

10:36AM Y28.00014 Low dimensional density of states in atomic layer deposited Al\textsubscript{2}O\textsubscript{3}on In\textsubscript{0.53}Ga\textsubscript{0.47}As. HAN-CHIN CHIU, L.T. TUNG, Y.H. CHANG, Y.J. LEE, C.C. CHANG, M. HONG, Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan, J. KWÓ, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — Atomic-layer-deposited (ALD) Al\textsubscript{2}O\textsubscript{3} dielectrics on In\textsubscript{0.53}Ga\textsubscript{0.47}As with short air exposure between oxide and semiconductor deposition has been demonstrated nearly ideal capacitance-voltage (C – V) characteristics with negligible frequency dispersion at flat-band and accumulation. A relationship of surface potential versus gate voltage derived by the excellent quasi-static C – V curve shows high efficiency of 63% for Fermi-level movement near the mid-gap. A low mean interfacial density of states (D\textsubscript{it}) \approx 2.5x10\textsuperscript{11} cm\textsuperscript{−2}eV\textsuperscript{−1} was determined using the charge pumping method, which was also employed to probe the depth profile of bulk trap density (N\textsubscript{bt}) and the energy dependence of D\textsubscript{it} measured at 50kHz: a low N\textsubscript{bt} \approx 7x10\textsuperscript{19} cm\textsuperscript{−2} and D\textsubscript{it} of 2-4x10\textsuperscript{11} cm\textsuperscript{−2}eV\textsuperscript{−1} in the lower half of the band-gap and a higher D\textsubscript{it} of \approx 10\textsuperscript{12} cm\textsuperscript{−2}eV\textsuperscript{−1} in the upper half of the band-gap. The employment of charge pumping method has given a more accurate determination of D\textsubscript{it}, which is usually overestimated using other commonly methods such as Terman, conductance, and high-low frequencies, due to the influence of weak inversion at room temperature.

10:48AM Y28.00015 Palladium and Palladium-Carbon Nanotube Composite Nanomechanical Resonator, SUNGWAN CHO, YOUNGDUCK KIM, JUNGHOO BAK, JUHYUNG LEE, SEUNGRAN LEE, KOOKRIN CHAR, SEUNGHUN HONG, YUN DANIEL PARK, School of Physics and Astronomy, Seoul National University — For its bio-compatibility, conductivity and optical reflectivity, metallic thin films are an attractive choice to realize multifunctional micromechanical resonators. However, moderate elastic properties of metallic thin films are ill suited for high frequency applications. Meanwhile, Carbon nanotubes have shown great potential with superior electrical and mechanical properties. Combined Metal-CNT nanolaminates have increased strengths and are less susceptible to onset of mechanical nonlinearity compared to equivalent metal beams without CNT. With palladium’s good affinity to CNT to further study the role of the metal-CNT interface, we realized doubly clamped beam and torsional resonators from Palladium and Palladium/CNT composite. Resonance frequencies were detected using optical modulation technique with different wavelength at room temperature.

Friday, March 20, 2009 8:00AM - 11:00AM
Session Y29 GMAG: Focus Session: Spin Liquids 333

8:00AM Y29.00001 Topological pairing of skyrmions and symmetry breaking in low-dimensional SU(N) antiferromagnets\textsuperscript{1}. ALEXEI KOLEZHUK, RWTH Aachen University — I study what happens to a so-called SU(N) antiferromagnet when the high SU(N) symmetry gets explicitly broken. Physically, such SU(N) antiferromagnets can be realized in cold atom systems in optical lattices (partially, the N=3 case corresponds to spin-1 bosons), and similar models might be possibly relevant for some magnetic materials like NiGa\textsubscript{S}\textsubscript{1}. I consider two perturbations breaking the SU(N) symmetry down to O(N) and SU(N-1), respectively, and study the phase diagram of the system. Breaking symmetry has a twofold effect: except favoring a certain type of order (spin-nematic or antiferromagnetic), it also affects the topological (Berry) phases. It is shown that the physically interesting case N=3 is very special: the effect of “topological pairing” of skyrmions leads to a change in the degeneracy of the disordered phase in case of SU(N) to O(N) perturbation, and the SU(N) to SU(N-1) perturbation brings the system into a critical phase.

\textsuperscript{1}Supported by the Heisenberg Program of DFG.

8:12AM Y29.00002 Cascade of quantum phase transitions in the spin-1/2 triangular-lattice antiferromagnet Cs\textsubscript{2}CuBr\textsubscript{4}\textsuperscript{1}. NATHANAELE FORTUNE, ADRIENNE WILSON-MUENCHOW, Smith College, SCOTT HANNAHS, National High Magnetic Field Laboratory, YASU TAKANO, University of Florida, YASUO YOSHIDA, University of Hamburg, TODD SHERLINE, Oak Ridge National Laboratory, TOSHIO ONO, HIKEAKU TANAKA, Tokyo Institute of Technology — In classical magnetic spin systems, geometric frustration leads to a large number of states of identical energy. We report here calorimetric and magnetocaloric evidence that in Cs\textsubscript{2}CuBr\textsubscript{4} — a geometrically frustrated Heisenberg S=1/2 triangular antiferromagnet — quantum fluctuations stabilize a series of gapped collinear spin states bounded by first-order transitions at simple increasing fractions of the saturation magnetization for fields directed along the c axis. Only the first of these quantum phase transitions has been theoretically predicted. We discuss how the higher fraction quantum states might arise and propose model spin arrangements. The Dzyaloshinskii-Moriya interaction breaks the symmetry when the magnetic field is directed along the triangular layers, providing one possible explanation for the directional dependence and the 1st order nature of the transitions.

\textsuperscript{1}Supported by awards from the Research Corporation, JSPS, Monakash and the NHMFL, funded by NSF and the State of Florida.
8:24AM Y29.00003 Dzyaloshinskii-Moriya interactions and non-magnetic impurities in the s=1/2 kagome antiferromagnet\textsuperscript{1}, IOANNIS ROUSOCHATZAKIS, SALVATORE MANMANA, Ecole Polytechnique Federale de Lausanne, Switzerland, ANDREAS LAEUCHLI, Max Planck Institut für Physik Komplexer Systeme, Dresden, Germany, BRUCE NORMAND, FREDERIC MILA, Ecole Polytechnique Federale de Lausanne, Switzerland — Motivated by recent NMR experiments\textsuperscript{1} on ZnCu$_2$(OH)$_6$Cl$_2$, we present an exact diagonalization study of the combined effect of non-magnetic impurities and Dzyaloshinskii-Moriya (DM) interactions in the s=1/2 Kagomé antiferromagnet. The magnetization response and the correlation matrix data reveal that the dimer freezing which occurs around the vacancy for D = 0 \[2,3\] (D is the magnitude of the DM vectors) persists up to D/J ≃ 0.07, above which a phase transition to the Q = 0 semiclusal 120° state\textsuperscript{4} takes place. Surprisingly however, the dimers next to the vacancy remain strong up to D/J = 2 – 3, i.e. well above the critical point. Implications for ZnCu$_2$(OH)$_6$Cl$_2$ will be discussed. 1. A. Olariu, et al., Phys. Rev. Lett. 100, 067202 (2008). 2. S. Dommange, et al., Phys. Rev. B 68, 224416 (2003). 3. A. Läuchli, et al., Phys. Rev. B 76, 144113 (2007). 4. O. Cépas, et al., Phys. Rev. B 78, 140405 (2008).

\textsuperscript{1}Swiss National Fund

8:36AM Y29.00004 Neel ordering and the stability of the spin 1/2 kagome lattice antiferromagnet in Zn-Paratacamite, MICHAEL J. LAWLER, Binghamton University, Cornell University, ERIK S. SORENSEN, McMaster University, YONG BAEK KIM, University of Toronto — Zn-Paratacamite is a rare spin 1/2 antiferromagnetic insulator with an ideal kagome lattice structure in part of its phase diagram. As a function of Zn doping, this material undergoes a structural distortion which relieves the frustration and introduces magnetic order in the ground state, though the precise nature of the order is not clear at this point. In this talk, I will present strong evidence for Neel ordering in the distorted phase of Zn-Paratacamite through the application of quantum Monte-carlo and exact diagonalization methods to the appropriate Heisenberg model. These numerical results strongly support a recent Schwinger-boson mean field theory of Zn-Paratacamite. Furthermore, our results indicate a large basin of stability of the ideal kagome lattice ground state in the presence of this type of distortion. This suggests that the ideal kagome ground state may be stable towards weak doping-induced distortion, though further studies of local effects may be necessary to make a firm conclusion.

8:48AM Y29.00005 Magnetization steps on the spin liquid ground state of the S = 1/2 kagome-like antiferromagnet Cu$_3$V$_2$O$_7$(OH)$_2$2H$_2$O, HIROYUKI YOSHIDA, YOSHIHIKO OKAMOTO, TAKASHI TAYAMA, TOSHIRO SAKAKIBARA, MASASHI TOKUNAGA, AKIRA MATSUO, YASUO NARUMI, KOICHI KINDO, MAKOTO YOSHIDA, MASASHI TAKIGAWA, ZENJI HIRAI, ISSP, Univ. of Tokyo, VOLTBOURTHITE COLLABORATION — The ground state of the S = 1/2 kagome antiferromagnet (KAFM) is expected to be a spin liquid with a finite spin gap $\Delta \sim J/2$. Here, we report the magnetic properties of S = 1/2 KAFM Cu$_3$V$_2$O$_7$(OH)$_2$2H$_2$O studied by magnetization, specific heat and V NMR measurements. Neither magnetic long-range order nor a spin gap has been detected down to 60 mK, in spite of a large antiferromagnetic interaction $J = 86$ K, suggesting a gapless spin liquid. Surprisingly, we observed three step-like increases in magnetization at $H_{S1} = 4.3$, $H_{S2} = 25.5$, and $H_{S3} = 46$ T, which implies that there exist at least four kinds of spin liquid or other quantum state under magnetic fields.

9:00AM Y29.00006 $^{69,71}$Ga NMR Probe of the Spin Dynamics in the Rare-Earth Kagomé Pr$_6$Ga$_5$SiO$_{14}$, LLOYD LUMATA, Department of Physics and National High Magnetic Field Laboratory, Florida State University, K.-Y. CHOI, Department of Physics, Chung-ang University, Seoul, South Korea, T. BESARA, M. R. HOCH, H. D. ZHOU, J. S. BROOKS, P. L. KUHNS, A. P. REYES, N. S. DALAL, C. R. WIEBE, NHMF/FSU — We report $^{69,71}$Ga nuclear magnetic resonance investigation of the spin dynamics in the rare-earth kagomé system Pr$_6$Ga$_5$SiO$_{14}$. We find that the spin-lattice relaxation rate $T_1^{-1}/T_2$ exhibits a peak around 30 K, below which the Pr$^{3+}$ spin correlation time $\tau$ shows novel field-dependent behavior consistent with a field-dependent gap in the excitation spectrum. The spin-spin relaxation rate $T_1^{-1}/T_2$ exhibits a maximum at a lower temperature (10 K) below which field-dependent power-law behavior close to $T^{2\alpha}$ is observed. These results point to the interplay of single-ion anisotropy and field-induced formation of nanoscale magnetic clusters consistent with recent neutron scattering measurements.

This work was supported in part by NSF DMR-0602859 and performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0084173, EIEG grant, by the State of Florida, and by the DOE.

9:12AM Y29.00007 Ba$_3$Cr$_2$O$_6$, a new non-Cu based quantum s=1/2 spin singlet system, MAIKO KOFU, Univ. of Virginia — Field-induced condensation of magnons has been experimentally observed in several weakly coupled quantum (s = 1/2) dimer systems that are based on Cu$^{2+}$ ions, such as TlCuCl$_2$ and BaCuSi$_2$O$_6$, and it has been adequately described by the Bose-Einstein condensation (BEC) theory. However, the robustness of such descriptions can only be truly evaluated with investigation into complementary materials, in particular materials that are based on non-Cu$^{2+}$ ions. Recently, a spin dimer system, BaCr$_2$O$_6$ has been found, where Cr$^{3+}$ (s = 1/2) ion with the unusual 5+ electronic valence forms quantum dimers along the c-axis and a frustrating triangular lattice in the ab-plane. Using elastic and inelastic neutron scattering measurements on single crystals and a powder sample, we have characterized the magnetic interactions to show that Ba$_3$Cr$_2$O$_6$ is indeed an excellent model system of weakly coupled quantum dimers\textsuperscript{[1]}. We have also investigate the field-induced condensation of magnons in this compound, using specific heat, bulk magnetization, and elastic neutron scattering measurements under an external magnetic field. The experimental results and comparison will be discussed.\textsuperscript{5}\textsuperscript{*}This work is in collaboration with J.-H. Kim, S. Ji, S.-H. Lee (University of Virginia), H. Ueda, Y. Ueda (ISSP, University of Tokyo), H. Nojiri (IMR, Tohoku University), B. Lake, K. Rule (Heinholz Centre Berlin).

\textsuperscript{[1]} M. Kofu et al., cond-mat/0809.5069 (2008).

9:48AM Y29.00008 BEC of triplon in the complex quantum spin liquid BaCuSi$_2$O$_6$, RAIVO STERN, NICPB, Tallinn, Estonia, STEFFEN KRAEMER, MLADEN HORTVATIC, GHMF, Grenoble, France, IVO HEINMÄA, ENNO JOON, NICPB, Tallinn, Estonia, CLAUDE BERTHIER, GHMF, Grenoble, France, TSUYOSHI KIMURA, Osaka University, Japan, JOEL MESOT, PSI, Switzerland — We present a $^{63,65}$Cu and $^{29}$Si NMR study of the quasi-2D coupled spin 1/2 compound BaCuSi$_2$O$_6$ in the magnetic field range 13-26 T and at temperatures as low as 50 mK. NMR data and neutron scattering experiments in the gapped phase reveal that below 90 K different in-dimer exchange couplings and different gaps ($\Delta_B/\Delta_A = 1.16$) exist in every second plane along the c-axis, in addition to a planar incommensurate (IC) modulation. $^{29}$Si spectra in the field induced magnetic ordered phase reveal that close to the quantum critical point at $H_{ic} = 23.35$ T the average boson density $\pi$ of the Bose-Einstein condensate (BEC) is strongly modulated along the c-axis with a density ratio for every second plane $\pi_A/\pi_B \approx 5$. An IC modulation of the local density is also present in each plane.

\textsuperscript{5}Supported by EU FP programs Euromagnet I & II, COST P16 “ECOM”, ESF HFM and Estonian Science Foundation.
10:00AM Y29.00009 High-Frequency EPR Studies of the Antiferromagnet Spin Dimer Compound \( \text{Ba}_3\text{Mn}_2\text{O}_8 \). CHANGHYUN KOO, STEPHEN HILL, Department of Physics, University of Florida, Gainesville, FL 32611; NHMFL and Department of Physics, FSU, Tallahassee, FL 32310. ERIC C. SAMULON, IAN R. FISHER, Geballe Laboratory for Advanced Materials and Department of Applied Physics, Stanford University, Stanford, CA 94305 — \( \text{Ba}_3\text{Mn}_2\text{O}_8 \) is a triangular lattice antiferromagnetic spin-dimer system based on pairs of spin \( S = 1 \) Mn\(^{2+} \) ions. In zero-field, \( \text{Ba}_3\text{Mn}_2\text{O}_8 \) possesses a singlet ground state. Meanwhile, application of a large magnetic field induces several ordered phases associated with the closing of gaps to the excited triplet and quintet states. Field orientation dependent high frequency electron paramagnetic resonance (HEPFR) measurements for a single crystal of \( \text{Ba}_3\text{Mn}_2\text{O}_8 \) have been carried out in fields up to 45 T using the hybrid magnet at the National High Magnetic Field Laboratory. Broad low-frequency transitions are observed in the field ranges close to \(-9 \) T to \(-32 \) T, suggesting inter-spin multiplet excitations. Sharper resonances are observed at higher frequencies, which persist to 42 T. Meanwhile, low-field studies provide information on the magnetic anisotropy of the system, which is of the easy-plane type with \( D = -0.375 \) K. We attempt to account for the observed HEPFR spectra in the context of a model recently developed to explain the magnetic properties of this compound [E. C. Samulon et al., Phys. Rev. B 77, 214441 (2008)].

10:12AM Y29.00010 \(^{135,137}\) Ba NMR study of condensed phase and critical behavior in \( S=1 \) spin dimer system \( \text{Ba}_3\text{Mn}_2\text{O}_8 \). STEVE SUH, W.G. CLARK, S.E. BROWN, UCLA, E.C. SAMULON, I.R. FISHER, Stanford, C.D. BATISTA, LANI, A.P. REYES, P. KUHNS, L.L. LUMATA, J.S. BROOKS, NHMFL — \( \text{Ba}_3\text{Mn}_2\text{O}_8 \) is a trigonal \( S = 1 \) spin dimer system, in which we have used \(^{135,137}\) Ba NMR spectroscopy and relaxation to study the static and dynamic properties of the field-induced phases and phase transitions to temperatures as low as 20mK, and with emphasis on magnetic fields up to 12T. Specifically, we report on the nature and variation of the order parameter in the condensed phases as well as the form of the spin lattice relaxation in the condensed phases, and compare to behavior anticipated for BEC and 3DXY universality classes. The temperature dependence of magnetization and the relaxation rate at the quantum critical point at \( H \sim 9T \) is also reported. For the case of the magnetization, a 3D to 2D crossover is evident, and shown consistent with calculations based on the magnon dispersion relations (M.B. Stone et. al, PRL 100, 237201 (2008)).

10:24AM Y29.00011 ABSTRACT WITHDRAWN —

10:36AM Y29.00012 The symmetry of the spin Hamiltonian in herbertsmithite, a spin-1/2 kagomé lattice. OREN OFER, AMIT KEREN, Physics Department, Technion, Israel Institute of Technology, Haifa 32000, Israel — We present magnetization measurements on oriented powder of \( \text{ZnCu}_2(\text{OH})_6\text{Cl}_2 \) along and perpendicular to the orienting field. We find a dramatic difference in the magnetization between the two directions. It is biggest at low measurement fields \( H \) or high temperatures. We show that the difference at high temperatures must emerge from Ising-like exchange anisotropy. This allows us to explain muon spin rotation data at \( T \rightarrow 0 \) in terms of an exotic ferromagnetic ground state.

10:48AM Y29.00013 Magnetic Excitations in the Stacked Quantum Magnets \( \text{NaNiO}_2 \) and \( \text{LiNiO}_2 \). J.P. CLANCY, B.D. GAULIN, J.P.C. RUFF, K.A. ROSS, G.J. VAN GASTEL, McMaster University, D.L. ABERNATHY, M.B. STONE, Oak Ridge National Laboratory — \( \text{NaNiO}_2 \) and \( \text{LiNiO}_2 \) are isostructural stacked triangular lattice quantum magnets, in which magnetism is conventionally thought to arise due to spin 1/2 moments carried by \( \text{Ni}^{3+} \) ions. Surprisingly, while \( \text{NaNiO}_2 \) undergoes a cooperative Jahn-Teller transition at 480K and magnetically orders below \( T_N \sim 23K \), \( \text{LiNiO}_2 \) undergoes a glass transition at \( T_g \sim 9K \) and remains disordered down to the lowest measured temperatures. The absence of long-range magnetic order in \( \text{LiNiO}_2 \) has been attributed to either geometric frustration caused by mixing of the Li and Ni sublattices, or orbital degeneracy due to the absence of a coherent Jahn-Teller distortion. We have performed time of flight neutron scattering measurements on polycrystalline samples of \( \text{NaNiO}_2 \) and \( \text{LiNiO}_2 \) using the wide Angular-Range Chopper Spectrometer (ARCS) at the SNS. Our measurements reveal previously unobserved magnetic excitations at relatively high energy transfers, which we associate with ferromagnetic spin waves mediated by in-plane interactions. We also find evidence of critical scattering in \( \text{NaNiO}_2 \) near the magnetic phase transition at \( T_N \). These results will be compared with previous measurements collected using the DCS at NIST.

Friday, March 20, 2009 8:00AM - 11:00AM — Session Y30 GMAG DMP: Focus Session: LAO/STO Interfaces 334

8:00AM Y30.00001 Coulomb Catastrophe and the Origin of the Sheet Carrier Density at the n-type LaAlO\(_3\)/SrTiO\(_3\) Interface: What do band calculations tell us?\(^1\). ZORAN POPOVIC, Institute for Nuclear Sciences, Belgrade, SASHI SATPATHY, University of Missouri, Columbia, RICHARD MARTIN, University of Illinois, Urbana — Transport measurements of the two-dimensional electron gas (2DEG) at the intrinsic n-type LaAlO\(_3\)/SrTiO\(_3\) interface have found a density of carriers much lower than expected from the “Coulomb catastrophe” arguments. From a detail density-functional study, we suggest how this discrepancy may be reconciled. We find that electrons occupy multiple subbands at the interface leading to a rich array of transport properties. Some electrons are confined to a single interfacial layer and susceptible to localization, while others with small masses and extended over several layers are expected to contribute to transport.

\(^1\)Work supported by the US Department of Energy; Ref: Z. Popovic, S. Satpathy, and R. M. Martin, Phys. Rev. Lett. (in press)

8:12AM Y30.00002 Quantum nature of two-dimensional electron gas confinement at LaAlO\(_3\)/SrTiO\(_3\) interfaces. KAROLINA JANICKA, Department of Physics and Astronomy, University of Nebraska Lincoln, JULIAN VELEV, Department of Physics, Institute for Functional Nanomaterials, University of Puerto Rico, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska Lincoln — Replace this text with your abstract body. The discovery of highly conducting interface between two insulating oxides LaAlO\(_3\) and SrTiO\(_3\) has attracted significant interest due to possible applications in all-oxide electronic devices. The two-dimensional electron gas (2DEG) formed at LaAlO\(_3\)/SrTiO\(_3\) interfaces exhibits extremely high mobility and high density of carriers. Stimulated by this discovery we perform density functional calculations to understand the mechanism controlling the confinement width of the two-dimensional electron gas (2DEG) at LaAlO\(_3\)/SrTiO\(_3\) interfaces. We find that the 2DEG confinement can be explained by the formation of metal induced gap states (MIGS) in the band gap of SrTiO\(_3\). These states are formed as the result of quantum-mechanical tunneling of the charge created at the interface due to electronic reconstruction. The penetration depth of the MIGS into the insulator is controlled by the lowest-decay-rate evanescent states of SrTiO\(_3\), as determined by its complex band structure. Our calculations predict that the 2DEG is confined in SrTiO\(_3\) within about 1 nm at the interface.

8:24AM Y30.00003 ABSTRACT WITHDRAWN —


Characterization tools that resolve spatially the physical properties and also detect spatial tiny changes of stoichiometry at the interface/surface of complex conductive-tip atomic force microscopy [1], electron energy loss spectroscopy [2] or low-temperature high-magnetic field measurements [3, 4], to characterize oxides. To characterize crucial aspects of these 2DEG such as the spatial extension as well as carrier density profiles, sophisticated techniques are required.

Contact to the 2DEG is relatively easy in this geometry since the current does not have to pass through the high band gap LAO layer. We have obtained a 2-D carrier density of 2x10^14 electrons/cm^2 at room temperature along with a mobility of 10 cm^2/Vs.

This work was supported by the DOE BES at the F. Seitz Materials Research Laboratory at the University of Illinois, Urbana.

9:00AM Y30.00006 Electrostatic doping in oxide heterostructures[1], ALEXANDER A. DEMKOV, JAEEKWANG LEE, NA SAI, The University of Texas — Recent experiments on perovskite heterostructures grown by methods ranging from molecular beam epitaxy to pulsed laser deposition suggest the existence of two dimensional electron gas of high mobility at the oxide/oxide interface, and even a possibility of a superconducting state. Both p-type and n-type interfaces have been reported. However, the origin of charge in these insulating materials is still under debate. We report a first-principles study of several heterostructures where we employ the internal filed in a polar oxide LaAlO$_3$ to demonstrate the possibility of the electrostatic doping, an effect similar to a well known polar catastrophe in e.g., III-V semiconductors. We use density functional theory at the LDA+U level. We mainly focus on the electronic structure of the oxide/oxide junctions. The results of our calculations suggest that once the critical thickness of the aluminate layer is reached the internal electric field is sufficient to produce the electrostatic doping. We will discuss simple estimates for the temperature of the superconducting transition and the role of oxygen-related defects such as vacancies in the electronic structure and thermodynamic stability of these fascinating oxide structures.

Supported by the NSF under CAREER grant DMR-0548182 and ONR under grant N00 154-06-1-0362

9:12AM Y30.00007 Nanoscale analysis of high-mobility electron gases at SrTiO$_3$ interfaces and surfaces, GERVASI HERRANZ, Institut de Ciencia de Materials de Barcelona, ICMAB-CSIC, Bellaterra, Spain — Electronic reconstructions or defects localized next to an interface between two oxides may lead to dramatic modifications of their physical properties. One intriguing example of such phenomena is the formation of high-mobility two-dimensional electron gases (2DEG) at the interface between LaAlO$_3$ and SrTiO$_3$ (STO), two insulating dielectric perovskite oxides. To characterize crucial aspects of these 2DEG such as the spatial extension as well as carrier density profiles, sophisticated techniques are required. Here I explain how we used the synergetic combination of different advanced characterization tools including depth-resolved positron annihilation spectroscopy, conductive-tip atomic force microscopy [1], electron energy loss spectroscopy [2] or low-temperature high-magnetic field measurements [3, 4], to characterize with nanometric space resolution high-mobility electron gases at STO interfaces and surfaces. Our results emphasize the relevance of using interface/surface characterization tools that resolve spatially the physical properties and also detect spatial tiny changes of stoichiometry at the interface/surface of complex oxide structures.


9:48AM Y30.00008 Band offsets between SrTiO$_3$ and LaAlO$_3$, KRISTOPHER E. ANDERSEN, Northern Arizona University, C. STEPHEN HELLBERG, Naval Research Laboratory — Although separately SrTiO$_3$ and LaAlO$_3$ are both band insulators, together a highly mobile, quasi-2D electron gas can form at their interface. Several mechanisms have been proposed to produce this electron gas, including the electrostatic divergence within LaAlO$_3$. A critical property in understanding this divergence is the valence band offset between SrTiO$_3$ and LaAlO$_3$. However, because the electrostatic potential can diverge, it is not clear where the valence band offset should be defined; an issue that may affect experimental band offset measurements. In this talk, the band offsets between SrTiO$_3$ and LaAlO$_3$ are presented within the framework of density functional theory. Both the layer projected density of states and macroscopically averaged potential are used to find the valence band offset for thin films and multilayers.

10:00AM Y30.00009 Transport and band profiles of MBE grown LaAlO$_3$/SrTiO$_3$, YARON SEGAL, J.H. NGAI, J.W. REINER, F.J. WALKER, C.H. AHN, Department of Applied Physics and Center for Research on Interface Structures and Phenomena, Yale University — Previously reported properties of the LaAlO$_3$/SrTiO$_3$ system showed strong dependence on growth parameters. This makes it difficult to identify the key physical quantities. To isolate the role of oxygen content, we grew LaAlO$_3$ films on SrTiO$_3$ using MBE. The thermal evaporation of MBE minimizes potential damage to the substrate and interface. The samples were then annealed at low temperature for a prolonged time, thus raising the oxygen content without damaging the structural integrity of the film. Transport and X-ray photoemission measurements were performed before and after annealing on films grown on both terminations of the substrate. Transport measurements show the in-plane conductivity decreases by several orders of magnitude upon annealing. A dependence on film thickness appears in certain oxygen content regimes, where it can be interpreted as being controlled by oxygen diffusion. Photoemission measurements reveal an intriguing band structure in the LaAlO$_3$ film. The termination of the SrTiO$_3$ determines the direction of apparent band bending, for which we discuss possible models. Our results imply that while transport behavior of this system is dominated by oxygen diffusion, the atomic details of the interface have a substantial impact on band structure.
10:12AM Y30.00010 Resonant Anomalous Synchrotron X-Ray Studies of LaAlO$_3$ Films on SrTiO$_3$(001)\(^\dagger\), DILLON FONG, TIM FISTER, MARIE-INGRID RICHARD, STEPHAN HRUSZKIEWYCZ, JEFFREY EASTMAN, PAUL FUOSS, Argonne National Laboratory, SUNG SEOK SEO, HO NYUNG LEE, Oak Ridge National Laboratory, ARGONNE NATIONAL LABORATORY TEAM — The high conductivity present at the interface between LaAlO$_3$ and TiO$_2$-terminated SrTiO$_3$(001) has been attributed to an electronic reconstruction [1] or atomic intermixing [2], both induced by the polar discontinuity. LaAlO$_3$ films with thicknesses equal to or thinner than a critical thickness (three unit cells [3]), however, can maintain the interface dipole, and no reconstruction (electronic or atomic) is expected. In this study, we employ resonant anomalous x-ray scattering at the Ti K-edge to investigate the structure and properties of the LaAlO$_3$ films both above and below the critical thickness. For films thicker than the critical thickness, an interfacial layer is observed to form. The structure and chemical properties of the interfacial layer as determined by both resonant scattering and x-ray spectroscopy will be discussed.

\(^\dagger\)This work is supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

10:24AM Y30.00011 Oxygen vacancy, charge doping, and polarization screening in LaAlO$_3$/SrTiO$_3$ interface\(^\dagger\), YUN LI, JAEJUN YU, Seoul National University — A high mobility electron gas has been observed in the n-type (TiO$_2$)/(LaO) interface between two insulators: non-polar SrTiO$_3$ (STO) and polar LaAlO$_3$ (LAO) and the mechanism of conductivity and dimensionality of electron gas at the interface have been intensively investigated in various experiments. There are two mechanisms suggested for the observed conductivity at the interface: electronic reconstruction and oxygen vacancy. We carried out density-functional-theory calculations to investigate the distribution of electron carriers for the n-type LAO/STO interfaces with and without oxygen vacancy. When no oxygen vacancy is present, the critical thickness of LAO film for conducting interface was found to be consistent with experiments. The induced carrier density at the interface without oxygen vacancy turns out to be an order of magnitude smaller than the one expected from the electronic reconstruction. This implies that the lattice polarization takes a significant role in charge screening. On the other hand, when oxygen vacancies are present, the vacancy-induced states are found to affect the carrier doping as well as the screening of polar electric field of LAO film. From the results, we propose that the upper limit of carrier doping should be 0.375 electrons per unit cell.

\(^\dagger\)Supported by BK21 FPRD, KOSEF, and KISTI.

10:36AM Y30.00012 The effect of strain on the SrTiO3/LaAlO3 heterointerface. C. TYLER DIGGANS, KRISTOPHER E. ANDERSEN, Northern Arizona University, C. STEPHEN HELLBERG, Naval Research Laboratory — Recent experiments have shown that it is possible to form a highly mobile, quasi-2D electron gas at the interface between SrTiO$_3$ and LaAlO$_3$. Although the origin of this effect is still debated, there is growing consensus that under certain growth conditions (e.g. high oxygen pressures) it is caused by the diverging electric potential within LaAlO$_3$ -the so-called polar catastrophe. One aspect of this system that has not been previously considered is the electric polarization of SrTiO$_3$, which can be effectively tuned by strain. This polarization can partially or fully compensate the diverging LaAlO$_3$ potential, and must be considered if SrTiO$_3$/LaAlO$_3$ is to be grown on a substrate such as Si. In this talk, an electrostatic model is presented to show how the polar catastrophe is modified by polarization within strained SrTiO$_3$. This model is supported by first-principles calculations on strained SrTiO$_3$/LaAlO$_3$ multilayers of varying thickness.

10:48AM Y30.00013 Polarization effects and the source of electrons in two-dimensional electron gas at insulating oxide heterointerfaces. H.W. JANG, D.A. FELKER, C.M. FOLKMAN, D.L. PROFITT, S.H. BAEK, M.S. RZCHOWSKI, C.B. EOM, University of Wisconsin-Madison, K. JANICKA, Y. WANG, M.K. NIRANJAN, E.Y. TSYM, University of Nebraska-Lincoln — The discovery of a two-dimensional electron gas (2DEG) at the heterointerface between insulating perovskite oxides LaAlO$_3$ and SrTiO$_3$ has stimulated intensive theoretical and experimental studies on the origin of the 2DEG. Empirically, the electron density has been found to be strongly dependent on the oxygen partial pressure during growth and the thickness of the polar LaAlO$_3$ layer. Understanding and controlling the source of the electrons in 2DEGs at oxide heterointerfaces is important for the optimization of their performance. In this talk, we will discuss electrical properties of heterointerfaces between various polar perovskites and SrTiO$_3$ fabricated by pulsed laser ablation. The importance of built-in electric fields due to polarization-induced charges, bandgap energy, and oxygen vacancies in the polar layers is highlighted using a simple analysis based on electrostatics. The experimental Hall data are then compared with the theoretical result from first-principles calculations.

Friday, March 20, 2009 8:00AM - 11:00AM —
Session Y31 GMG: Focus Session: Neutron Scattering

8:00AM Y31.00001 Anomalous spin-waves in triangular lattice antiferromagnets\(^\dagger\), MIKE ZHITOMIRSKY, CEA, Grenoble, SASHA CHERNYSHCHEV, UC Irvine — The distinct features of spin-wave excitations in the triangular-lattice antiferromagnet are (i) a finite lifetime at zero temperature due to spontaneous two-magnon decays, (ii) strong renormalization of magnon energies \(\epsilon_k\) with respect to the harmonic result, and (iii) logarithmic singularities in the decay rate \(\Gamma_k\). Detailed quantitative results are obtained for the magnon spectrum of the spin-1/2 model using both the on-shell and off-shell solutions of the Dyson’s equation. In the low-energy limit magnons remain well-defined excitations but with anomalous decay rates. At high energies, magnons are heavily damped by decay rates reaching \((2\Gamma_k/\epsilon_k) \sim 0.3\). The on-shell solution shows logarithmic singularities in \(\Gamma_k\) with the concomitant jump-like discontinuities in \(\epsilon_k\) along certain contours in the momentum space. Such singularities are even more prominent in the magnon spectral function \(\Lambda(k,\omega)\). Although the off-shell solution removes such log-singularities, the decay rates remain strongly enhanced. We also discuss the role of higher-order corrections and show that such singularities may lead to incomplete disappearance of the spectrum in the vicinity of certain k-points. We conclude that magnon decays and singularities must be prominent in a wide class of noncollinear antiferromagnets.

\(^\dagger\)Supported by the DOE under DE-FG02-04ER46174 (SC)

8:12AM Y31.00002 Two Dimensional Correlations and Field Induced Order in the Pyrochlore Ferromagnet Yb$_2$Ti$_2$O$_7$, KATE ROSS, J.P.C. RUFF, B.D. GAULIN, McMaster University, C.P. ADAMS, St Francis Xavier University, J.S. GARDNER, NCNR, H.A. DABKOWSKA, McMaster University, Y. QIU, UMD / NCNR, J.R.D. COPLEY, NCNR — The rare earth pyrochlore magnets are of intense current interest due to their often unconventional magnetic behaviour. The pyrochlore lattice, which is occupied by the magnetic ions in such materials, is the 3D archetype for geometric frustration. We have studied the frustrated pyrochlore magnet, Yb$_2$Ti$_2$O$_7$, in single crystal form using time-of-flight neutron scattering. Our study confirms the presence of diffuse rods of scattering, which indicate unexpected 2D magnetic correlations in this cubic system. The diffuse scattering is measured both above and below a previously reported first order transition at \(T_c \approx 240\text{K}\). Although rod-like scattering persists below \(T_c\), three dimensional correlations develop, indicating a build-up of interplane correlations. Yet Yb$_2$Ti$_2$O$_7$ continues to resist long range order down to \(\sim 50\text{K}\). We have discovered, however, that the application of a small magnetic field along the [110] direction readily induces a long range ordered magnetic state, as evidenced by well defined spin wave excitations. We will present a magnetic phase diagram for Yb$_2$Ti$_2$O$_7$ based on the results of this study.

\(^\dagger\)Work supported by NSERC
Excitations within the field-induced ordered phases in Ba$_3$Mn$_2$O$_7$ lead to a quasi-two-dimensional behavior. We also present magnetic field-dependent neutron scattering measurements examining long range order and excitations within the field-induced ordered phases in Ba$_3$Mn$_2$O$_7$.

This state consists of coexisting short and long range orders[3], and that both orders can be destroyed by the application of modest magnetic fields to be selected either by unusual anisotropic interactions, or via thermal and/or quantum fluctuations in an example of order-by-disorder [1,2]. Recently, we have shown that this state consists of coexisting short and long range orders[3], and that both orders can be destroyed by the application of modest magnetic fields[3]. This disordering of the magnetic system involves a seemingly continuous quantum critical point at $\mu_0H_c \sim 1.6$ Tesla [3]. The properties of the induced quantum paramagnetic state, and the dependence of these properties on the direction of applied field will be discussed. I will also make comparisons with a recent theoretical treatment of Er$_2$Ti$_2$O$_7$[2].

2McClarty et al. arXiv:0810.2483v2

Spin waves and quantum criticality in the frustrated XY pyrochlore antiferromagnet Er$_2$Ti$_2$O$_7$ - Jacob Ruff, McMaster University - Geometrically frustrated magnetism in the three dimensional pyrochlore lattice often gives rise to unconventional magnetic states at low temperatures. The effective elimination of leading energetic terms via geometric cancellation allows weak perturbations to ultimately determine the behaviour of a magnetic material. In this talk, I will describe the manifold of low energy states in the antiferromagnetic XY pyrochlore Er$_2$Ti$_2$O$_7$, as measured by the time-of-flight neutron scattering technique. In zero applied magnetic field, the ground state is purported to be selected either by unusual anisotropic interactions, or via thermal and/or quantum fluctuations in an example of order-by-disorder [1,2]. Recently, we have shown that this state consists of coexisting short and long range orders[3], and that both orders can be destroyed by the application of modest magnetic fields [3]. This disordering of the magnetic system involves a seemingly continuous quantum critical point at $\mu_0H_c \sim 1.6$ Tesla [3]. The properties of the induced quantum paramagnetic state, and the dependence of these properties on the direction of applied field will be discussed. I will also make comparisons with a recent theoretical treatment of Er$_2$Ti$_2$O$_7$ [2].

2McClarty et al. arXiv:0810.2483v2

Recent neutron scattering results from Gd-based pyrochlore oxides - Jason Gardiner, Indiana University - In my presentation I will present recent results that have determined the spin-spin correlations in the geometrically frustrated magnets Gd$_2$Sm$_2$O$_7$ and Gd$_2$Ti$_2$O$_7$. This will include polarised neutron diffraction, inelastic neutron scattering and neutron spin echo data. One sample of particular interest is Gd$_2$Sm$_2$O$_7$ which is believed to be a good approximation to a Heisenberg antiferromagnet on a pyrochlore lattice with exchange and dipole-dipole interactions. Theoretically such a system is expected to enter long range ordered ground state known as the “Palmer Chalker” state [1]. We show conclusively, through neutron scattering data, that the system indeed enters an ordered state with the Palmer-Chalker spin configuration below $T_c = 1$ K [2-3]. Within this state we have also observed long range collective spin dynamics, spin waves. This work has been performed in collaboration with many research groups including G. Ehlers (SNS), R. Stewart (ISIS).


Electric Control of Spin Chirality in Multiferroic Ni$_3$V$_2$O$_8$ - Ivelisse Cabrera, Johns Hopkins University, Michel Kenzelmann, University of Neutron Scattering, ETH Zurich and Paul Scherrer Institute, Gavín Lawes, Wayne State University, OKSana Zaharko, Laboratory for Neutron Scattering, ETH Zurich and Paul Scherrer Institute, Collins Broholm, Johns Hopkins University — We discuss electric control of spin chirality in the magnetically frustrated multiferroic Ni$_3$V$_2$O$_8$ through polarized magnetic neutron diffraction. Cooling to the cycloidal magneto-electrostatic phase in an electric field $E$ causes the incommensurate Bragg reflections to become neutron spin polarizing, the sense of neutron polarization reversing with $E$. Comprehensive polarized neutron diffraction measurements establish the chiral nature of the long range ordered spin configuration and its response to $E$. Concomitant evolution of chiral and ferroelectric domains is observed by comparing polarized neutron diffraction data to pyroelectric current measurements and hysteresis under different poling conditions [1].

2Work at JHU was supported by NSF through Grant No. DMR-0706553.
3Work at JHU was supported by NSF through Grant No. DMR-0706553.

8:36AM Y31.00004 Spin waves and quantum criticality in the frustrated XY pyrochlore antiferromagnet Er$_2$Ti$_2$O$_7$ - Jacob Ruff, McMaster University - Geometrically frustrated magnetism in the three dimensional pyrochlore lattice often gives rise to unconventional magnetic states at low temperatures. The effective elimination of leading energetic terms via geometric cancellation allows weak perturbations to ultimately determine the behaviour of a magnetic material. In this talk, I will describe the manifold of low energy states in the antiferromagnetic XY pyrochlore Er$_2$Ti$_2$O$_7$, as measured by the time-of-flight neutron scattering technique. In zero applied magnetic field, the ground state is purported to be selected either by unusual anisotropic interactions, or via thermal and/or quantum fluctuations in an example of order-by-disorder [1,2]. Recently, we have shown that this state consists of coexisting short and long range orders[3], and that both orders can be destroyed by the application of modest magnetic fields [3]. This disordering of the magnetic system involves a seemingly continuous quantum critical point at $\mu_0H_c \sim 1.6$ Tesla [3]. The properties of the induced quantum paramagnetic state, and the dependence of these properties on the direction of applied field will be discussed. I will also make comparisons with a recent theoretical treatment of Er$_2$Ti$_2$O$_7$ [2].


8:24AM Y31.00003 Beyond Simple Bilayers in the Triangular Lattice Dimer compound Ba$_3$Mn$_2$O$_7$ - Matthew Stone, Mark Lumsden, Oak Ridge National Laboratory, Sung Chang, NIST, Eric Samulon, Stanford University, Cristian Bátísta, Los Alamos National Laboratory, Kirrily Rule, Bensec, Eric Ressoüche, Beatrice Grenier, Ill, Jan Fisher, Stanford University — We present single crystal inelastic neutron scattering measurements of the $S = 1$ dimerized quasi-two-dimensional antiferromagnet Ba$_3$Mn$_2$O$_7$. The singlet-triplet dispersion reveals nearest-neighbor and nextnearest-neighbor ferromagnetic interactions between adjacent bilayers that compete against each other. Although the interbilayer exchange is comparable to the intrabilayer exchange, this additional frustration reduces the effective coupling along the $c$ axis and leads to a quasi-two-dimensional behavior. We also present magnetic field-dependent neutron scattering measurements examining long range order and excitations within the field-induced ordered phases in Ba$_3$Mn$_2$O$_7$.

9:36AM Y31.00007 CEF groundstate of the frustrated quantum magnets SrRE$_2$O$_4$ (RE = Dy, Ho), A. Desilets-Benoit, A. D. Bianchi, Dep. de physique, Universite de Montreal, Montreal, QC, Canada, V. Pomsakushin, B. R. Hansen, LNS, PSI, Villigen, Switzerland, M. Kenzelmann, LDM, PSI, Villigen, Switzerland, R. J. Cava, Dept. Chemistry, Princeton University, Princeton, NJ, USA — We have measured the crystalline electric field (CEF) niveaus of the magnetic ions in the frustrated quantum magnets SrRE$_2$O$_4$ with RE = Dy and Ho by inelastic neutron scattering. SrRE$_2$O$_4$ crystallizes in a $pmn$ structure, which as four in-equivalent rare earth sites, leading to a large degree of geometrical frustration. Fitting a CEF level scheme to the experimental data has allowed us to determine the CEF ground state of this system.

9:48AM Y31.00008 Dynamics of excitations in a one-dimensional Bose liquid, Maxim Khodas, Brookhaven National Laboratory — The dynamical structure factor $S(q, \omega)$ of interacting 1D liquid is studied. This quantity has become experimentally accessible in the recent experiments on cold atoms and neutron scattering off spin chains. We find power law non-analyticities $S(q, \omega) \propto (\omega - \epsilon_{1,2}(q))^{-\mu(q)}$ at the kinematical thresholds characterized by the momentum dependent exponents evaluated in a broad range of parameters.

10:24AM Y31.00009 Magnetic properties of LuFe$_2$O$_4+y$, Fan Wang, Jungho Kim, University of Toronto, G Xu, S.M. Shapiro, G.D. Gu, Brookhaven National Laboratory, Y. Lee, Yonsei University, Y.-J. Kim, University of Toronto — LuFe$_2$O$_4+y$ (LFO) has been drawing much attention as a potential multiferroic compound. We show that the oxygen stoichiometry plays an important role in determining the magnetic properties of LFO. The sample with excess oxygen shows two magnetic transitions at 236K and 228K. The transition at 236K is a paramagnetic to ferrimagnetic transition, and below 228 K the system enters a spin glass phase. The DC magnetization shows strong time and history dependence, while the AC susceptibility exhibits dynamic scaling behaviour similar to that of canonical spin glass systems. This spin glass behaviour seems to disappear in the more stoichiometric sample. In this second sample, long range ferrimagnetic ordering has been observed with neutron scattering experiments. Our X-ray scattering on single crystal and X-ray powder diffraction experiments both show there is a structural change around 170K, which seems to be responsible for an observed low field anomaly. When a small magnetic field is applied, magnetization is only turned on during heating the sample. With large applied field, a metamagnetic transition was observed.
10:36AM Y31.00010 Phonon renormalization of the Néel transition in KCuF$_3$. J.C.T. LEE, S. YUAN, University of Illinois, Urbana-Champaign, A. RUSYDI, National University of Singapore, S. SMADICI, L. COOPER, E. FRADKIN, P. ABBAMONTE, University of Illinois, Urbana-Champaign — Critical magnetic fluctuations in the one-dimensional antiferromagnet KCuF$_3$, in the form of diffuse scattering around the magnetic (001) Bragg peak, have been studied with resonant soft x-ray scattering. Using x-rays near the Cu $L_3$ edge to exploit the $2p \rightarrow 3d$ dipole transition, the (001) was directly observed at temperatures ranging from 23K to above the transition temperature ($T_N \approx 43$K). Notably, the phase transition exhibits hysteresis, with $T_N$ sensitive to whether the sample was cooled or heated prior to measurement. This suggests that the phase transition is weakly first order, as might be expected by a transition renormalized by phonons. The temperature dependence of the coherence length and the diffuse scattering, as well as the role played by Jahn-Teller phonons in the transition are discussed.

1This work was supported by US DOE grants DE-FG02-07ER46453 and DE-FG02-06ER46285.

10:48AM Y31.00011 The influence of magnetic field on Cu(tn)Cl$_2$ - two-dimensional quantum magnet with Néel ground state. A. ORENDACOVA, M. ORENDAC, L. SEDLAKOVA, A. FEHER, Centre Low Temp. Phys., P. J. Safarik Univ. and SAS, Kosice, Slovakia, K. SIEMENSMEYER, A. BUCHSTEINER, Helmholtz Zentrum Berlin, Germany, J. S. XIA, L. YIN, M.W. MEISEL, NMHFL and Dept. Phys., Univ. Florida — AC susceptibility and neutron elastic scattering experiments were performed on Cu(tn)Cl$_2$ [1] to explore the origin of a field induced anomaly previously observed in specific heat below 1 K and in finite fields up to 7 T [2]. Isothermal AC susceptibility scans, made down to 40 mK and in fields up to 10 T, confirmed and extended the B vs. T phase diagram obtained from the specific heat data. Neutron spectra of a polycrystalline sample studied down to 0.5 K in B = 0 and 4 T did not reveal any magnetic peaks expected below 1 K and indicated a slight change of (200) nuclear peak intensity induced by the magnetic field. The possible reasons of the absence of a phase transition to ordered state will be discussed. [1] V. Zelenak et al., Inorg. Chem. 45 (2006) 1774. [2] A. Orendacova et al., in preparation.

Friday, March 20, 2009 8:00AM - 10:36AM — Session Y32 GMAG DMP FIAP: Focus Session: Current-Induced Magnetic Switching 336

8:00AM Y32.00001 Effect of spin diffusion in the polarizer on current-induced magnetic switching. SCOTT BUTTON, SERGEI URAZHDIN, West Virginia University — Current-induced magnetic switching of a nanomagnet occurs due to the spin transfer torque exerted by current spin-polarized by another ferromagnet. Efficient switching is generally achieved by enhancing the polarizing properties of the latter. However, calculations show that switching is affected not only by the polarizing properties of the polarizer, but also by the electron diffusion in this layer [1,2]. To test the effects of spin diffusion in the polarizer on current-induced switching, we performed measurements of magnetic multilayer nanopillars with three different structures of the polarizing magnetic layer: a thick Co layer, a thin Co layer, and a bilayer consisting of a thin Co layer and a strongly spin-flipping FeMn alloy. In the pillars with a thick Co polarizer, the switching currents dramatically increase below 130 K, while the magnetoresistance exhibits a nonmonotonic dependence on temperature with a peak at 130 K. In contrast, the samples with a thin Co polarizer exhibit weak monotonic dependencies of switching and magnetoresistance on temperature. We discuss the implications of our results for our understanding of spin-dependent diffusion in magnetic multilayers. [1] A.A. Kovalev, A. Brataas, and G.E.W. Bauer, Phys. Rev. B 66, 224424 (2002). [2] Zhang, P.M. Levy, and A. Fert, Phys. Rev. Lett. 88, 236601 (2002).

1Supported by NSF DMR-0747609 and a Cottrell Scholarship from Research Corporation

8:12AM Y32.00002 Spin transfer torque switching of Co nanoparticles. HAN ZOU, Department of Physics and Astronomy University of Delaware, XIAOJUN WANG, YI JI, Department of Physics and Astronomy University of Delaware — Spin transfer torque effect has potential application in Magnetic Random Access Memory (MRAM) devices as a way to address the memory elements. Most spin transfer studies are based on patterned multilayer thin films with 100 nm lateral dimension. In this work, we demonstrate the feasibility of the spin transfer switching of a few cobalt nanoparticles with a diameter of < 5 nm at 4.2 K. The motivation arises from the prospect of device miniaturization and the capability to manipulate an individual magnetic nanoparticle. We use a multilayer thin film Co/100nm/Co/10nm/Co/3nm/Co/0.5nm/Au/2nm. The 0.5 nm Co layer is not continuous, and it consists of isolated Co particles formed due to surface tension. A mechanical point contact is formed on the multilayer film at 4.2K. By varying the size of the contact, the number of nanoparticles underneath a point contact can be controlled between ~5 and ~50. Hysteric loops in $dV/dI$ measurements clearly indicates spin-transfer switching. The $dV/dI$ curves are qualitatively different between point contacts involving only few particles (5-10) and those involving many particles (40-50).

1This work is supported by University of Delaware Research Foundation (UDRF) and U.S. DOE Grant No. DE-FG02-07ER46374.

8:24AM Y32.00003 Stochastic Resonance Driven by Spin Torque. XIAO CHENG, CARL BOONE, JIAN ZHU, ILYA KRIVOROTOV, University of California Irvine, UNIVERSITY OF CALIFORNIA IRVINE TEAM — Application of a microwave ac current to a spin valve gives rise to a rectified voltage due to magnetization dynamics driven by ac spin torque. We study the effect of dc current bias on these dynamics in spin valves with superparamagnetic free layers. We observe large enhancement of the rectified voltage (up to two orders of magnitude) along a line in the dc current - magnetic field phase diagram of the system. This enhancement arises from large-amplitude nonlinear dynamics of magnetization of the free layer induced by the combined action of ac and dc spin torques. For small out-of-plane external magnetic field, the enhanced rectified signal is observed at low frequencies (~1GHz) of the ac drive. This signal enhancement arises from adiabatic stochastic resonance of magnetization of the free layer driven by ac spin torque. For large out-of-plane magnetic field, the rectified signal enhancement is found at the ac drive frequencies of several GHz. We interpret this new type of large-amplitude high-frequency dynamics as non-adiabatic stochastic resonance of magnetization. Temperature-dependent measurements of the rectified signal confirm the stochastic resonance nature of the observed phenomena.
8:36AM Y32.00004 Reduction of spin-torque switching currents by partially canceling the free layer demagnetization field. LUQIAO LIU, TAKAHIRO MORIYAMA, DAN RALPH, ROBERT BUHRMAN, CORNELL UNIVERSITY TEAM — A small switching or excitation current is crucial for the successful application of spin torque (ST) in magnetic memory and on-chip oscillator devices. The required ST current for an in-plane-polarized nanomagnet is proportional to its effective field, within which the out-of-plane component (H_z) dominates. This large H_z, however, does not contribute to the thermal stability of the free layer. So it will be of great advantage if we can reduce H_z. Co/Ni multilayer structures have been shown to exhibit perpendicular anisotropy and we have precisely controlled the thickness of these multilayer components so that this crystalline anisotropy can be used to cancel the demagnetization field, reducing H_z to a value comparable to the in-plane geometry-dependent coercive field. In comparison to a control sample with a relatively higher H_z and the same magnetic volume, we find that the low H_z sample has much smaller ST reversal currents in both the quasi-state thermally activated and short pulse reversal regimes. The fact that the free layer magnetization lies in plane and the fixed layer(s) can be conventional magnetic material(s) makes it more tractable to deal with the dipole coupling between the free and reference layers, and should also facilitate the incorporation of this approach in high performance ST devices that utilize magnetic tunnel junctions.

8:48AM Y32.00005 Effects of rf current on critical field for magnetization reversal in spin torque devices. WENYU CHEN, SYLVIA FLOREZ, JORDAN KATINE, MATTHEW CAREY, LIESL FOLKS, BRUCE TERRIS, Hitachi Global Storage Technologies — Current induced switching assisted by rf current has recently been observed in spin torque devices at low temperature [1, 2]. This effect allows control of spin transfer induced magnetization reversal through the frequency of an injected rf current. In this study, the effects of the rf current injection on critical field for magnetization reversal in spin valve junctions have been investigated. Measurements were conducted at room temperature, and the magnetic field was applied along the easy axis of the junction. An rf current was injected into the nanojunction at various frequencies ranging between 1 and 20 GHz. The dynamic resistance, dV/dI, was measured as a function of the rf frequency, power and the dc bias current while ramping the magnetic field. The rf current injection was observed to change the critical field for free layer magnetization reversal when the intrinsic spin-transfer-induced dynamics is frequency-locked with the injected rf. The results will be discussed in the context of macrospin models of spin transfer in metallic spin valve structures. [1] S. H. Florez et al. Phys. Rev. B 78, 184403 (2008) [2] Y.-T. Cui et al. Phys. Rev. B 77, 214440 (2008)

9:00AM Y32.00006 A Three Terminal Approach to Spin-Torque Written MRAM Cells, PATRICK BRAGANCA, Cornell University/Hitachi Global Storage Technologies — Magnetic random access memory (MRAM) is a potentially superior alternative to silicon-based memories due to a combination of properties including non-volatility, fast read/write times, and low power consumption. Future MRAM technologies have been considered which use the spin transfer effect as a mechanism for bit element writing. Here, a spin polarized current passing through a ferromagnetic element is used to reverse its moment via an exchange of angular momentum, as opposed to the magnetic fields from remote write lines used in more conventional toggle MRAM [1]. However, the large current densities required for spin transfer reversal create significant barrier wearout issues in the magnetic tunnel junctions (MTJs) used as bit elements. One possible solution is to develop a nanopillar structure where a third electrode can be made to any point within a thin-film multilayer stack, substantially enhancing the versatility of the device by providing the means of applying independent electrical biases to two separate parts of the device. Using experimental results and micromagnetic simulations, I will discuss a joint magnetic spin valve/tunnel junction structure sharing a common free layer nanomagnet contacted by this third electrode [2]. A spatially nonuniform spin-polarized current flowing into the free layer via the low-resistance spin valve path can reverse the magnetic orientation of the free layer as a consequence of the spin torque effect, by nucleating a reversal domain at the spin injection site that propagates across the free layer. The free layer magnetic state can then be read out separately via the higher-resistance magnetic tunnel junction. This three-terminal structure provides a strategy for developing high performance spin-torque MRAM cells which avoids the need to apply a large voltage across a MTJ during the writing step, thereby enhancing device reliability, while retaining the benefits of a high-impedance MTJ for read-out.


9:36AM Y32.00007 Invariant Form of the Spin-Transfer Switching Condition, INTI SODEMANN, YAROSLAV BAZALY, Department of Physics and Astronomy, University of South Carolina, USA — Conventional spin-transfer (ST) device with one fixed and one free layer is considered in the macrospin approximation for the case of constant driving current. The expression for the critical current capable of pushing the free layer magnetization out of the local energy minimum is obtained in an invariant form. It is found that the relevant quantity is the divergence of the spin-transfer torque, and not the strength of the torque itself. This shows that there is no essential difference between current induced switching in collinear and non-collinear geometries. The result further provides a qualitative picture of the influence of ST torque angular dependence on the switching current and allows to understand when the Slonczewski spin polarization coefficient g(θ) can, or cannot be approximated by a constant. We discuss the implications of the derived formulas for the engineering of low current devices.

9:48AM Y32.00008 Exchange assisted spin transfer torque switching, XI CHEN, Physics Department, University of Minnesota, RANDALL VICTORA, Electrical Engineering Department, University of Minnesota — The main challenge in the application of spin transfer torque switching is the high current required to reverse the magnetization. We propose a composite structure containing soft and hard magnetic layers that significantly lowered the switching current. The dynamic phase diagram of the structure is studied using a macrospin model, with Landau-Lifshitz-Gilbert equation including a spin-torque term. It is shown that the anisotropy of the hard layer, by using multiple soft layers with graded anisotropy, a further reduction can be achieved. We also show that the switching current grows linearly with the damping constant in the soft layer. This means that a low damping, soft material can facilitate the reversal of the hard layer and reduce the switching current by over an order of magnitude.

10:00AM Y32.00009 Structural Characterization of Spin-Torque Oscillators, SARAH C. PARKS, K. LI, A. HAUSER, J. E. THOMPSON, J. CIRALDO, J. EMERICK, J. LUCY, F. Y. YANG, E. JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — The discovery of current-induced magnetodynamics in giant magnetoresistive (GMR) trilayers promises a novel platform for microwave electronics. A key factor in determining the potential of this platform remains the development of nanoscale fabrication techniques, typically resulting in either nanopillar or point-contact geometries. As a result, a considerable technical barrier to further progress is the fidelity of current nanoscale patterning techniques. In an effort to address this challenge, we present the results of development efforts aimed at fabricating prototype point-contact spin torque oscillator (PC-STO) structures with a focused ion beam (FIB). The flexibility of FIB-based nanofabrication allows in situ cross sectional imaging of contact structure, and these results are correlated with DC magnetotransport. This fabrication approach enables the rapid generation of structures in arbitrary geometries, and in conjunction with cross-sectional imaging promises increased control of device to device variation and the development of novel PC-STO structures.

1Partial support for this research provided by the Ohio State University Institute for Materials Research and NSF ECCS Grant No. 0726133
10:24AM Y32.00011 All Spin Digital Circuits, BEHTASH BEHIN-AEIN, Purdue University / NSF Network for Computational Nanotechnology (NCN), DEEPANJAN DATTA, Purdue University, SAYEEF SALAHUDDIN, UC Berkeley, SUPRIYO DATTA, Purdue University — Switching of a magnetic free layer using spin polarized current has been demonstrated in Magnetic Tunnel Junction (MTJ) devices. Currently MTJ's are being studied for memory and microwave oscillator applications. The purpose of this talk is to explore a modified MTJ where a clock pulse via the fixed layer facilities the switching of the free layer in accordance with a weak field provided by an input magnet in the form of a spin current. Based on the Landau-Lifshitz-Gilbert equation (LLG) augmented with spin torque functions, we show the switching energy and the switching time of the free layer which indicates the possibility of very low power digital logic applications. Ordinary digital circuits store information in the form of capacitor charges that communicate through electrical interconnects. The purpose of this paper is to show that modified MTJ's can be the basis for all spin digital circuits. Our primary objective is to stimulate proof of concept experiments that could usher in a whole new set of devices suitable for spintronic circuits.

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Session Y33 DCMP: Nanowires and Quantum Dots 403

8:00AM Y33.00001 Digital Wires, BENNY BROWN, UC Davis, ALFRED HUBLER, UIUC — We study hardware implementations of cellular automata as reliable, adjustable, and secure commination lines. We discuss energy efficient digital wires on a nano-scale, all-optical digital wires, and digital wires as power lines and present performance data of a prototype digital wire, a six cells wide and ten cells long Boolean network. We show that digital wires have the following advantages: (i) Fixed pulse shape (pulses have a rectangular shape with a constant height and a constant width and produce no echos); (ii) Robust against electric smog. Digital wires based on semiconductor technology are effectively inert against electro-magnetic radiation, except for low-frequency radiation (heat) and high frequency radiation (X-rays). Digital wires based on plasma technology have in addition a very high tolerance for heat and X-rays. In digital wire the pulse speed can be rapidly adjusted. Signals on digital wires can be encrypted. Some digital wires can be used as general purpose computers. The data and the code are the input of the wire. Then both travel along the wire and ‘collide’. The collision is the computation. The result travels to the end of the wire, for further processing, as parallel input by a CPU, an actuator, or another digital wire.

8:12AM Y33.00002 ABSTRACT WITHDRAWN

8:24AM Y33.00003 Renormalization of the dephasing by zero point fluctuations, SWARNAJ BAN-DOPADHYAY, Physics Department, Norwegian University of Science and Technology, NO-7491, Trondheim, Norway, DORON COHEN, Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel — One of the most fundamental properties of an quantum particle is to maintain its phase-coherence. When an quantum particle is coupled to a fluctuating environment its wave-function gets phase-randomised. During the last decade a controversy has emerged in the mesoscopic literature regarding the role of zero-point-fluctuations (ZPF) in low temperature dephasing. We propose an exactly solvable model for dephasing due to short range scattering with environmental modes in dephasing at low temperature. Unlike the Caldeira-Leggett model where the interaction is with an homogeneous fluctuating field of force, here we consider the environment consisting of infinitely many localized fluctuating modes with (say) Ohmic spectral function and the interaction is local as in ‘s-scattering’. We find that in low temperature ZPF can enhance the inelastic cross-section. Our study shows [Phys. Rev. B 77, 155438 (2008)] we need finite temperature to see the effect. Thus indirectly ZPF might contribute to the dephasing at low temperature.

8:36AM Y33.00004 Helical [110] gold nanowires make longer linear atomic chains, EDGARD AMORIM, EDISON DA SILVA, Unicamp — Experiments performed on nanowires (NWs) synthesized by electron beam irradiation technique have shown that gold NWs formed along the [110] direction become helical when the NWs are sufficiently thin [1]. Moreover, helical and other non-crystalline structures have been theoretically predicted to other few metals [2]. Our study using tight-binding molecular dynamics show that gold NWs formed along the [110] direction reconstuct upon stress to form helical structures. We discuss this formation and our results seem to indicate that an intrinsic mechanism is responsible for the formation of the helical structure. These helical NWs evolve on stretching to form linear atomic chains (LACs) and because they do not form symmetrical tips, the NWs produce longer LACs than other NWs. We use ab initio calculations to study the NW obtained from the tight-binding simulations at stages close to rupture and compare LAC distances obtained with both methods. Furthermore, we investigate the electronic structure of the NW close to rupture [3].


8:48AM Y33.00005 Hall effect detection of time-reversal symmetry breaking under AC driving, ALEXEI CHEPELIANSKII, SOPHIE GUERON, Univ. Paris-Sud, CNRS, UMR 8502, F-91405, Orsay, France, FREDERIC PIERRE, ANTONELLA CAVANNA, BERNARD ETIENNE, Laboratoire de Photonique et de Nanostructures (LPN)-CNRS, ro ute de Nozay, 91460 Marcoussis, France, HELENE BOUCHAT, Laboratoire de Physique des Solides, Universite Paris Sud, Orsay France, GROUPE DE PHYSIQUE MESOSCOPIQUE TEAM, LABORATOIRE DE PHOTONIQUE ET DE NANOSTRUCTURES COLLABORATION — In a four terminal sample microscopic time-reversibility leads to symmetry relations between resistance measurements where the role of current and voltage leads are exchanged. These reciprocity relations are a manifestation of general Onsager-Casimir symmetries in equilibrium systems. We investigate experimentally the validity of time-reversal symmetry in a GaAs/Ga1-xAlxAs Hall bar irradiated by an external AC field at zero magnetic fields. For inhomogeneous AC fields we find strong deviations from reciprocity relations and show that their origin can be understood from the the billiard model of a Hall junction. Under homogeneous irradiation the symmetry is more robust indicating that time-reversal symmetry is preserved.

9:00AM Y33.00006 On time-dependent counting statistics of mesoscopic electron transport, WOLFGANG BELZIG, University of Konstanz — Full counting statistics (FCS) has emerged as a key concept to understand quantum transport in mesoscopic systems like heterostructures, quantum wires, and quantum dots. The knowledge of the FCS not only enables to predict all measurable zero-frequency quantities accessible via charge detection, but also allows to identify the elementary transport events and the correlations between them. We demonstrate this concept for a standard quantum point contact between normal and/or superconducting leads under dc- and ac-bias. [M. Vanevic, Yu. V. Nazarov, W. Belzig, Phys. Rev. Lett. 99, 076601 (2007)] Finally we address the question, how these concepts can be applied to time-resolved current measurements. [A. Bednorz and W. Belzig, Phys. Rev. Lett. 101, 206803 (2008)]
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Session Y34 DCMP: Superconducting Devices and Applications 404

8:00AM Y34.00001 Designing electron refrigerators for improved cooling with an expanded thermal model. GALEN O’NEIL, ERIK LARSON, CU Boulder/NIST Boulder, JOEL ULLOM, NIST Boulder — Normal-metal/insulator/superconductor (NIS) tunnel junctions can act as refrigerators below 1K. Biasing the junction such that only thermally excited electrons have energy higher than the superconducting gap causes selective tunneling which cools the normal metal electrode. Because of their small size, low mass, and absence of moving parts, NIS refrigerators are an attractive cooling technology for space and industrial applications. We have demonstrated temperature reductions of 100mK from bath temperatures near 300mK. For example, we operated a superconducting x-ray detector at 160mK with a cryostat bath temperature of 260mK by using NIS junctions for the additional cooling. We will show a more complete thermal model of a large area NIS refrigerator accounting for quasiparticle injection, diffusion, and imperfect trapping. Using this model to guide NIS refrigerator design we expect to achieve our goal of cooling from 300mK to 100mK.

8:12AM Y34.00002 ABSTRACT WITHDRAWN –

8:24AM Y34.00003 Nanomechanical parametric amplification and oscillation via electrostatic coupling to Cooper-pair box. JUNHO SUH, MATT LAHAYE, Caltech, PIERRE ECHTERNACH, Jet Propulsion Laboratory, KEITH SCHWAB, Cornell University, MICHAEL ROUKES, Caltech — Nanomechanical resonator coupled to a Cooper-pair box exhibits frequency modulation as a function of the gate voltage when the qubit is adiabatically tuned. We utilize this effect to demonstrate mechanical degenerate parametric amplification and oscillation. Gain above 30dB and self-oscillation is observed. This technique could provide an efficient way to enhance the force sensitivity in the measurement of coupled dynamics of nanomechanical resonator modes and a solid state qubit.

8:36AM Y34.00004 Back-action and self-oscillation in the Double Pump Josephson Parametric Amplifier (DPA) , ARCHANA KAMAL, ADAM MARBLESTONE, MICHEL H. DEVORET, Yale University — Josephson Parametric amplifiers are the most promising candidates for reaching the quantum limit of amplification at RF frequencies. The DPA employs 2 pumps. The dual pumps ensure separation between the signal and the pump frequencies, which is necessary to observe delicate effects, such as self-oscillations. We present the model of the DPA. Our calculations are based on Input-Output Theory, and can easily be generalized to any coupled system involving parametric interactions. We analyze the operation of the device, taking into account the feedback introduced by the reaction of the signal amplification on the pump power and we compute various response functions - signal/idler gain, internal gain, and steady state signal response. To account for this back-action between signal and pump, we adopt a mean-field approach and self-consistently explore the boundary between amplification and self-oscillation. The potential of the DPA for quantum-limited measurements and as a squeezer is also discussed.

8:48AM Y34.00005 Detection and Reset Dynamics of Superconducting Nanowire Single Photon Detectors1, ANTHONY ANNUNZIATA, Yale University, ORLANDO QUARANTA, University of Salerno, DANIEL SANTAVICCA, JOEL CHUDOW, LUIGI FRUNZIO, Yale University, AVIAD FRYDMAN, Bar Ilan University, MICHAEL ROKOS, Yale University and IBM Research, DANIEL PROBER, Yale University — We investigate the single photon detection and reset mechanisms in superconducting nanowires, which have received recent, widespread attention for use in applications requiring fast optical and near infrared photon counting. These devices are fabricated from ultra-thin Nb and NbN films and read out by measuring short (~1 ns) transient voltage spikes that result from the localized suppression of superconductivity by an absorbed photon. We find that intrinsic electro-thermal instabilities necessitate a low impedance (<50 ohms) readout circuit for stable resetting to the superconducting state after detecting a photon. The actual impedance needed depends on the detailed physical properties of the device. We also investigate the detection mechanism and report the dependence of detection efficiency on the temperature and dc bias current as well as on film disorder, from which we present a model of the detection mechanism.

1This work is supported by NSF - EPDT, NSF - Graduate Research Fellowship, and IBM research.

9:00AM Y34.00006 Measurements of a YBCO superconducting quantum interference filter with planar ion-damaged Josephson junctions1, STEVEN M. ANTON, SHANE A. CYBART, STEPHEN M. WU, JOHN CLARKE, R.C. DYNES, University of California, Berkeley — We have fabricated a two dimensional series-parallel array of 565 × 28 YBa2Cu3O7−δ thin film ion damage Josephson junctions. The loop areas were varied incommensurately from 28.5 to 90 µm2 so that the response of the current-biased array to an applied magnetic field is a prominent peak in voltage centered at zero field. We measured voltage versus applied magnetic field characteristics for several static bias currents at different temperatures. Additionally, we measured current-voltage (I-V) characteristics of the array with no applied magnetic field at several temperatures. To fit the I-V characteristics, we assumed that each parallel section of the array could be modeled as a single resistively shunted junction with critical currents following a normal distribution. Fitting the summed voltage contributions of the parallel sections to measurements of the array, we computed the resistance and critical current mean and spread. The standard deviation of these critical currents was 15 percent at 74 K.

1This work was supported by AFOSR, and by DOE through the LBNL Molecular Foundry.

9:12AM Y34.00007 Cryogenic Broadband Impedance-Matched Absorptive Microwave Filters . DANIEL SLICHTER, OFER NAAMAN, IRFAN SIDIQI, Quantum Nanoelectronics Lab, UC Berkeley — We report Johnson noise and S parameter measurements of a broadband impedance-matched low pass microwave filter consisting of a section of lossy stripline transmission line. The thermal noise power generated by the filter was measured in the frequency band of 1.2 GHz - 1.8 GHz at temperatures from 30 mK to 300 mK. The noise power was comparable to that of a 50Ω reference load held at the same temperature and measured with the same microwave measurement chain using a cryogenic mechanical switch. Transmission measurements on a filter with f_dB = 1.3 GHz show that the filter’s cutoff characteristics remain essentially unchanged between room temperature and 20 mK. The filters are robust to thermal cycling and are simple to manufacture. We have used these filters to obtain low Cooper pair temperatures in high-bandwidth microwave measurements on superconducting devices.
bilayers by treating the Al surface with an atomic nitrogen beam. Under optimum nitridation conditions the resultant analytical scanning transmission electron microscopy (STEM) with electron energy-loss spectroscopy (EELS) to investigate thin AlN layers formed on Nb/Al ultra-thin aluminum nitride (AlN) barrier layers can result in Josephson Junctions (JJ’s) with both very high critical current densities and low sub-gap leakage.

Josephson tunnel junctions have long been used as sensitive magnetic flux detectors. NanoSQUIDs, which use submicron weak link junctions for enhanced flux coupling, are attractive candidates for magnetic measurements of molecules. We present a novel method for nanoSQUID readout which involves embedding the SQUID in a superconducting transmission line cavity operating at microwave frequency. The magnetic flux dependence of the total SQUID inductance modulates the cavity resonant frequency; these frequency changes are determined using microwave reflectometry. This dispersive microwave measurement allows detection of changes in magnetic flux at submicrosecond timescales without creating dissipation in the vicinity of the molecule. Moreover, we can exploit the Josephson nonlinearity of the nanoSQUID for bifurcation amplification to enhance sensitivity. Optimization of the nanoSQUID design and cavity parameters for maximizing detector sensitivity and bandwidth is discussed. We also discuss the various sources of noise in this measurement scheme and how to minimize their impact. This work is supported by AFOSR and USDOE.

10:00AM Y34.00011 Single-artificial-atom lasing using a voltage-biased superconducting charge qubit, ROBERT JOHANSSON, RIKEN, SAHEL ASHHAB, RIKEN, University of Michigan, ALEXANDRE ZAGOSKIN, Loughborough University, FRANCO NORI, RIKEN, University of Michigan — We consider a system composed of a single artificial atom coupled to a cavity mode. The artificial atom is biased such that the most dominant relaxation process in the system takes the atom from its ground state to its excited state, thus ensuring population inversion. Even under this condition lasing cannot be suppressed if the relaxation rate is larger than a certain threshold value. Using simple transition-rate arguments and a semiclassical calculation, we derive analytic expressions for the lasing suppression condition and the state of the cavity in both the lasing and suppressed-lasing regimes. The results of numerical calculations agree very well with the analytically derived results. Our analysis and results are relevant to the recently realized superconducting artificial-atom laser. [arXiv:0803.1209]

10:12AM Y34.00012 A scanning SQUID microscope for imaging high-frequency magnetic fields, C. P. VLACHACOS, CNAM, Department of Electrical and Computer Engineering, University of Maryland College Park and the Laboratory of Physical Sciences, F. C. WELLSTOOD, Center for Nanophysics and Advanced Materials and Joint Quantum Institute, Physics Department, University of Maryland College Park, J. MATHIEWS, Physical Optics Corporation — We have developed a large-bandwidth scanning SQUID microscope in order to spatially image high frequency magnetic fields. By using a hysteric Nc-dc-SQUID and a pulsed sampling technique, rather than a non-hysteretic SQUID and a flux-locked loop, we have overcome the bandwidth limitations of existing scanning SQUID microscopes, which typically only image below about 1 MHz. The microscope allows for non-contact time-varying magnetic field images to be taken of room temperature samples with time steps down to 50 ps and spatial resolution ultimately limited by the size of the SQUID to about 10 μm. Towards this end, results will be presented on the design, development, and operation of a cryo-cooled 4.2 K scanning SQUID microscope with a bandwidth of dc to 3 GHz and a sensitivity of about 52.4 nT per sample.

10:24AM Y34.00013 The Josephson Microwave Photomultiplier1, BRENDAN OSBERG, JAY GAMBITTA, FRANK WILHELM, Institute for quantum computing — The current lack of single microwave photon counters as opposed to microwave amplifiers has become a problematic omission in the toolkit of available circuit QED devices. Hence, we propose a microwave photo-multiplier based on a modified phase qubit. Such a system, trapped in the metastable state, can be activated over its potential energy barrier by an incoming photon, creating an avalanche effect analogous to current photo-diodes. Linear coupling of the junction flux with the radiation field, in the weak damping regime, permits photodetection from an arbitrary quantum source in the GHz range. We model this device theoretically and investigate its sensitivity, bandwidth, efficiency, and dark-count rate using the Langevin stochastic differential equations and a path integral approach.

1This work supported by the Natural Sciences and Engineering Research Council of Canada, and by the Ontario Ministry of Training, Colleges and Universities.

10:36AM Y34.00014 Transport Properties of a Hybrid SET-SQUID Device in Tunable Dissipative Environment, SHUCHAO MENG, JEFFREY QUILLIAM, CHAS MUGFORD, Department of Physics and Astronomy and Institute for Quantum Computing, University of Waterloo, Waterloo, ON, N2L 3G1, ANDY SACHRAJDA, Institute for Microstructural Sciences, NRC, 1200 Montreal Road, Ottawa, ON, K1A 0R6, JAN KYCIA, Department of Physics and Astronomy and Institute for Quantum Computing, University of Waterloo, Waterloo, ON, N2L 3G1 — We will present measurements of transport properties of a new type of superconducting device, designed to allow a fully adjustable Hamiltonian with charge term, Josephson coupling term, and dissipation term. This device consists of a superconducting Single Electron Transistor (SET) and two Superconducting Quantum Interference Devices (SQUIDs). A 2D electron gas embedded 90nm below the substrate surface provides a tunable dissipative environment. A small magnetic field can be applied to drive this hybrid device from the strong Josephson coupling regime to the SET regime. Dissipation and temperature dependence of the switching current out of the zero-voltage state show different characteristics for different settings of competition between Josephson coupling and charging energy.
and Vortex Dynamics 405

superconducting phase diagram (Tc, Hc2) on Ba(Fe1−xCox)2As2 single crystals. The upper critical field anisotropy diminishes with temperature and has an unusual temperature dependence, (ii) Hc2(T = 0) for this compound may easily approach fields of 75 tesla. 1

Work performed at the National High Magnetic Field Laboratory supported by the NSF, by the State of Florida, and by the DOE

Friday, March 20, 2009 8:00AM - 11:00AM —

Session Y35 DMP: Focus Session: Iron Pnictides and Other Novel Superconductors XVI: Hc2 and Vortex Dynamics 405

8:00AM Y35.0001 Fluorine Doping Effect On Hc2 and Rh In LaFeAsO1−xFx . Y. KOHAMA, S. RIGGS, F. BALAKIREV, M. JAIME, Los Alamos National Laboratory, Y. KAMIHARA, T. ATAKE, M. HIRANO, H. HOSONO, Tokyo Institute of Technology — The iron arsenide superconductors discovered earlier this year have attracted much interest, and some families showing high-Tc have been identified. LaFeAsO (La: lanthanide) is the first copper-free family of compounds with Tc exceeding 50 K. Here, we present the first systematic study of Hc2 and Rh in the wide fluorine doping region (LaFeAsO1−xFx , x = 0, 0.25, 0.05, 0.07, 0.11 and 0.14). We found that Hc2 increases monotonically with decreasing x, while the superconducting phase diagram (Tc, x) displays the classic dome-shaped structure. Furthermore, the shape of Hc2(T) depends strongly on x. This, according to Gurevich’s model, suggests a multiband electronic structure. The Hall resistivity for non-superconducting samples x = 0, 0.025 show a non-linear magnetic field dependence, which also supports a multiband electronic structure interpretation. In addition, the estimated low-field limit of the Hc2 for x = 0, 0.025 detect a gap opening at the structural transition and magnetic transition. The evidence for multiband electronic structure links these materials to the famous multiband superconductor MgB2 rather than high-Tc cuprates.

8:12AM Y35.0002 Upper critical fields of NdFeAsO1.8F0.2 single crystal1. J. JAROSZYNSKI, F. HUNTE, L. BALICAS, YOUN-JUNG JO, IVANA RÀCEVIC, A. GUREVICH, D.C. LARBALESTIER, F.F. BALAKIREV, NHMFL, L. FANG, P. CHENG, Y. JIA, H.H. WEN, NLS CAS — We present measurements of the resistivity and the upper critical field Hc2 of NdFeAs O1.8F0.2 single crystals in strong DC and pulsed magnetic fields up to 45 T and 60 T, respectively. We found that the field scale of Hc2 is comparable to ~ 100 T of high Tc cuprates. Hc2(T) parallel to the c-axis exhibits a pronounced upward curvature similar to what was extracted from earlier measurements on polycrystalline samples. Thus this behavior is indeed an intrinsic feature of oxypnictides, rather than manifestation of vortex lattice melting or granularity. The orientational dependence of Hc2 shows deviations from the one-band Ginzburg-Landau scaling. The mass anisotropy decreases as T decreases, from 9.2 at 44 K to 5 at 34 K. We discuss to what extent different pairing scenarios can manifest themselves in the observed behavior of Hc2, using the two-band model of superconductivity. The results indicate the importance of paramagnetic effects on Hc2(T), which may significantly reduce Hc2(0) as compared to Hc2(0) ~ 200 – 300 T based on extrapolations of Hc2(T) near Tc down to low temperatures.

1Work performed at the National High Magnetic Field Laboratory supported by the NSF, by the State of Florida, and by the DOE

8:24AM Y35.0003 Determination of anisotropic Hc2 in (Ba0.55K0.45)Fe2As2 single crystals1. C. H. MIELKE, M. M. ALTARAWNEH, K. COLLAR, Los Alamos National Laboratory, N. NI, S. L. BUD’KO, P. C. CANFIELD, Ames Laboratory, NHMFL-PFF TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY, IOWA STATE UNIVERSITY TEAM — The radio frequency penetration depth was measured in SmFeAsO(O1−xFx)2 single crystals in strong DC and pulsed magnetic fields up to 45 T and 60 T, respectively. We found that the field scale of Hc2 is comparable to ~ 100 T of high Tc cuprates. Hc2(T) parallel to the c-axis exhibits a pronounced upward curvature similar to what was extracted from earlier measurements on polycrystalline samples. Thus this behavior is indeed an intrinsic feature of oxypnictides, rather than manifestation of vortex lattice melting or granularity. The orientational dependence of Hc2 shows deviations from the one-band Ginzburg-Landau scaling. The mass anisotropy decreases as T decreases, from 9.2 at 44 K to 5 at 34 K. We discuss to what extent different pairing scenarios can manifest themselves in the observed behavior of Hc2, using the two-band model of superconductivity. The results indicate the importance of paramagnetic effects on Hc2(T), which may significantly reduce Hc2(0) as compared to Hc2(0) ~ 200 – 300 T based on extrapolations of Hc2(T) near Tc down to low temperatures.

1LANL LDRD-20070013, DoE DE-AC02-07CH11358, NSF-DMR 0602859, DoE DMR-0654118

8:36AM Y35.0004 Thermodynamic estimation of the upper critical field slope of doped Sm-FeAsO from fluctuation conductivity in the critical regime . MARINA PUTTI, ILARIA PALLECCHI, CARLO FANCIULLI, MATTEO TROEPANO, MAURIZIO FERRETTI, ALBERTO MARTINELLI, ANDREA PALENZONA, CARLO VERDEGHINI, CNR-INFM-LAMIA and University of Genova, Via Dodecaneso 33, 16146 Genova, Italy — We measure magnetotransport in SmFeAs(O1−xFx)2 polycrystalline samples up to 28 T and we extract the upper critical fields, using different criteria. Due to fluctuation effects, not negligible magnetoresistance and resistivity not saturating to a residual value at Tc, Hc2 values turn out to be strongly criterion-dependent. In order to circumvent this problem, we propose a thermodynamic estimation of the upper critical field slope dHc2/dT based on the analysis of conductivity fluctuations in the critical regime at high fields. Indeed, in this regime we find evidence of a two-dimensional lowest Landau level (LLL) scaling for applied fields larger than μ0H baff ∼ 8T, which allows to extract a high field slope as large as -12T/K for the optimally doped sample SmFeAsO(O0.55K0.45)2. A comparison of the fluctuation behavior with that of high-Tc cuprates indicates that this Hc2,LLL value may be related to the Hc2 and κ values higher than those of cuprates.

8:48AM Y35.0005 Upper critical field in Ba(Fe1−xCo1−x)2As2 and FeSe1−yTe1−y compounds. CHIARA TARANTINI, JAN JAROSZYNSKI, JIANYI JIANG, ALEX GUREVICH, DAVID C. LARBALESTIER, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA, RONGYIN JIN, ATHENA S. SEFAT, MICHAEL A. MCGUIRE, BRIAN C. SALES, DAVID G. MANDRUS, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — We report Hc2 measurements in high magnetic field up to 31 T on Ba(Fe1−xCo1−x)2As2 and FeSe1−yTe1−y pnictide compounds for different doping levels. Both materials exhibit a very high upper critical fields and unconventional temperature dependences of Hc2(T) with the extremely high slopes dHc2/dT from 10 to 30 T/K near Tc and a relatively low anisotropy: γ = Hc2(Tc) / Hc2(T) for the doped ternary compound and γ ≈ 1.1 ± 1.2 for the binary one. The observed temperature dependences of Hc2(T) and the high Hc2 values well above the BCS paramagnetic limit indicate the importance of the Zeeman pairbreaking effects in these compounds.
9:00AM Y35.00006 Thermodynamic Determination of the Upper Critical Field and Anisotropy of Ba$_{1.0}$K$_{0.4}$Fe$_2$As$_2$ Single Crystals

WAI-K. KWOK, ULRICH WELP, RUOBING XIE, ALEXEI KOSHELEV, JOHN SCHLUETER, JIONG HUA, Institute of Physics, Chinese Academy of Sciences, Beijing, China — We present anisotropic heat capacity measurements of the upper critical field of Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ single crystals in fields up to 8 Tesla. In zero-magnetic field a clear step in the heat capacity is observed at $T_c \sim 36K$. Using an entropy conserving construction we determined the transition temperatures in applied fields and the upper critical field slopes $dH_c^2(0)/dT = -6.5 \text{T/K}$ and $dH_c^2(4.5)/dT = -17.4 \text{T/K}$, the latter showing record high critical field slope near $T_c$.

9:12AM Y35.00007 Inter- and intra-granular current properties of iron pnictide superconductors

AKIYASU YAMAMOTO, ANATOLII POLYANSKII, JIANYI JIANG, FUMITAKE KAMETANI, MARINA PUTTI, CHIARA TANGANTINI, FRANK HUNTE, JAN JAROSZYNSKI, ERIC HELLSTROM, ALEX GUREVICH, DAVID LARBALESTIER, National High Magnetic Field Laboratory — The iron pnictide superconductors have very high upper critical field $B_c(0)$ of possibly over 100 T for 1111 and 50-70 T for 122. We have recently shown [1,2] that polycrystalline 1111 samples exhibit electromagnetic granular behavior, perhaps in an analogous way to that seen now to be intrinsic to the HTS cuprates. Detailed investigation is proceeding in parallel with serious efforts to make more single phase samples, since it appears that all present polycrystalline oxypnictides are multi-phase. In particular we are using magneto-optical imaging to study the local variation of current density and then performing detailed microstructural analysis by SEM, TEM and orientation analysis to understand intergranular current flow. At the present time we see that samples are multi-phase, often with a grain boundary wetting phase, but even so the global $J_c$ attains 1000-4000 A/cm$^2$, some 10-40 times that seen in single phase YBCO randomly polycrystalline Nb-Ti. On the other hand, very high intra-grain critical current owing to the strong pinning of Nb-Ti is observed in the Co doped Ba122 pnictide. We will report on our latest results on the inter- and intra-granular current properties in the high-$T_c$ pnictides. [1] A. Yamamoto et al., Appl. Phys. Lett. 92, 252501 (2008). [2] A. Yamamoto et al., Supercond. Sci. Technol. 21, 095008 (2008).

9:24AM Y35.00008 Magneto-optical imaging of flux distribution in single crystal Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ of various doping level $x$.

ERICK C. BLOMBERG, Ames laboratory and Department of Physics & Astronomy, Iowa State University, P. PROMMAPAN, M. A. TANATAR, V. C. KOGAN, N. NI, S. L. BUD’KO, P. C. CANFIELD, R. PROZOROV — Near optimal doping of Ba(Fe$_{0.93}$Co$_{0.07}$)$_2$As$_2$ crystals measured the uniform superconductivity and vortex properties similar to high-$T_c$ cuprates.[1] In this contribution, single crystals of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with the measured doping level $x=3.8\%$, 4.7\%, 5.8\%, 7.4\%, 10\%, and 11.8\%, covering all regimes - from underdoped to overdoped were studied using real-time magneto-optical imaging. Inhomogeneity of the superconducting state as well as field and temperature dependencies of the magnetic induction distribution were analyzed. Superconductivity is homogeneous at all except for the highest doping level. The results are correlated with macroscopic transport and magnetic measurements.

9:36AM Y35.00009 ABSTRACT WITHDRAWN

9:48AM Y35.00010 Similarity Between Fe-based Pnictide Superconductors and High-$T_c$ Cuprates Revealed by the Irreversible Magnetic Behavior in the Vortex State

RUSLAN PROZOROV, M.A. TANATAR, C. MARTIN, R.T. GORDON, E.C. BLOMBERG, P. PROMMAPAN, V.G. KOGAN, N. NI, M.E. TILLMAN, S.L. BUD’KO, P.C. CANFIELD, Ames Laboratory and Department of Physics & Astronomy, Iowa State University — Static and dynamic measurements of DC magnetization and direct real-time magneto-optical imaging have revealed unconventional vortex behavior in NdFeAsO$_{x}$Fe$_2$O$_{1-x}$ and Ba(Fe$_{0.93}$Co$_{0.07}$)$_2$As$_2$ single crystals with superconducting transition temperature at 24 K. With detailed understanding of the flux pinning mechanism in the iron-based superconducting materials. Static and dynamic behavior of vortices are investigated by transport, bulk magnetization, and quantitative magneto-optical imaging techniques, while high resolution analytical TEM is used to investigate the structural inhomogeneity down to atomic level. Frequent flux jump, and enhanced flux pinning at elevated magnetic field, corresponding to the “fish tail” in magnetization hysteresis, are often observed. We will discuss the relationship between the flux pinning behavior and structural detailed properties in this and other related superconducting materials.

10:00AM Y35.00011 Flux Pinning and Structural Inhomogeneity in Superconducting BaFe$_{1.8}$Co$_{0.2}$As$_2$ Single Crystals

QIANG LI, JUAN ZHOU, Brookhaven National Lab, JIUFENG TU, City College of New York, YUHANG REN, Hunter College, CUNY, LINJUN LI, YONGKANG LUO, HANG CHEN, GUANZHANG CAO, ZHU’AN XU, Zhe Jiang University — We report coordinated studies of flux pinning behavior and structural inhomogeneity in BaFe$_{1.8}$Co$_{0.2}$As$_2$ single crystals with superconducting transition temperature at 24 K, in order to understand the flux pinning mechanism in the iron-based superconducting materials. Static and dynamic behavior of vortices are investigated by transport, bulk magnetization, and quantitative magneto-optical imaging techniques, while high resolution analytical TEM is used to investigate the structural inhomogeneity down to atomic level. Frequent flux jump, and enhanced flux pinning at elevated magnetic field, corresponding to the “fish tail” in magnetization hysteresis, are often observed. We will discuss the relationship between the flux pinning behavior and detailed structural properties in this and other related superconducting materials.

10:12AM Y35.00012 Thermally-activated and temperature-independent magnetic relaxation in aligned grains of NdFeAsO(F)

JAMES R. THOMPSON, Dept. of Physics, University of Tennessee and Oak Ridge National Laboratory, Y. L. ZUEV, D. K. CHRISTEN, E. D. SPECHT, R. JIN, B.C. SALES, M. A. MCGUIRE, A. SEFAT, D. G. MANDRUS, Oak Ridge National Laboratory — We have studied flux creep in a magnetically-aligned powder of NdFeAsOF and found it to be strikingly similar to the situation in cuprates. The magnetic relaxation rate $S = \ln M(t)/\ln t$ is linear in temperature at low temperatures. There is an extrapolated finite creep rate of about $S = 0.02$ at $T = 0$, indicative of a quantum tunneling of vortices under energy barriers. This quantum creep rate is field-independent. From the temperature-dependent creep data we have obtained activation energy as a function of persistent current density, $U(J)$. Comparison with existing creep theories will be made.

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1This work was supported by the US Department of Energy, BES-Materials Sciences, under Contract DE-AC02-06CH11357.


on-going torque magnetometry measurements are expected to check the validity of this interpretation. We developed and used a scheme that allows for the calculation of the essential transport parameters, such as the trap DOS, in an unambiguous controlled conditions. This was done by temperature-dependent gated four-terminal measurements on pentacene thin-film transistors prior to and after controlled oxygen exposure. We studied the influence of oxygen on the electronic trap states in a pentacene thin film kept under highly controlled conditions. These results demonstrate the possibility of dynamic field-guided patterning of molecule-on-metal systems. We also showed that applied electric fields can be employed to enhance or retard the diffusivity of FePc molecules which the arrangement of active molecules is fixed or can be controlled and the contact-molecule-contact system exhibits desirable electronic properties. Fe (II) logic and memory devices, sensors, fuel cells, and solar cells. The implementation of practical molecular electronic devices requires molecule-on-metal systems in which the arrangement of active molecules is fixed or can be controlled and the contact-molecule-contact system exhibits desirable electronic properties. We suggest that it is attributable to the distinctive electronic structure of the iron-arsenic compounds. Our measurements indicate that in contrast to the assumptions based on the cuprates, reduced dimensionality is not a prerequisite for “high-temperature” superconductivity.

Supported by DoE grant “Science in 100 T”.

8:12AM Y36.00002 Oxygen-related traps in pentacene thin films: Energetic position and implications for transistor performance, WOLFGANG KALB, Laboratory for Solid State Physics, ETH Zurich, Switzerland, KURT MATTENBERGER, BERTRAM BATLOGG — We studied the influence of oxygen on the electronic trap states in a pentacene thin film kept under highly controlled conditions. This was done by temperature-dependent gated four-terminal measurements on pentacene thin-film transistors prior to and after controlled oxygen exposure. We developed and used a scheme that allows for the calculation of the essential transport parameters, such as the trap DOS, in an unambiguous way. The results are free from parasitic contact artifacts. Oxidation of pentacene in light leads to a peak of trap states centered at 0.28 eV from the mobility edge, with trap densities of the order of $10^{18}$ cm$^{-3}$. The measurements reveal how these traps affect the key device parameters, i.e. subthreshold performance and field-effect mobility. The study supports the assumption of a mobility edge for charge transport, and contributes to a detailed understanding of an important degradation mechanism of organic field-effect transistors.

8:24AM Y36.00003 Grazing-incidence X-ray Diffraction of Tetracene Thin Films on Hydrogenated Si(001) Substrate, DE-TONG JIANG, ANDREW TERSIGNI, Dept. of Physics, University of Guelph, CHANG-YONG KIM, Canadian Light Source, JUN SHI, Dept. of Physics, University of Guelph, ROBERT GORDON, Physics Dept., Simon Fraser University, NING CHEN, Canadian Light Source, XIAORONG QIN, Dept. of Physics, University of Guelph — Ex situ grazing-incidence X-ray diffraction (GIXD) and wide angle Bragg diffraction have been performed on UHV epitaxially grown tetracene thin films on H/Si(001)-2×1 substrates. The in-plane lattice of the crystalline films were characterized by 2D reciprocal space imaging of the in-plane (11), (12) and (20) GIXD diffraction spots and the out-plane lattice of the crystalline films were characterized by the wide angle Bragg diffraction. The thickness of the tetracene films ranged from 1.2 monolayer (ML) to 15 ML. H/Si(001)-2×1 substrates with different surface roughness were used. The results indicate that the film structure characteristics are strongly influenced by the substrate conditions and under favorable conditions the homogeneous thin-film phase could dominate the growth up to about 8 ML. The implications of the results to the growth mechanisms and to thin film electronics applications will be discussed.
corresponding changes in the conductivity which occur when organic absorbates are present. By increasing the coverage from sub-monolayer to multilayer, it
is possible to see doping of the underlying Ag layer, as well as conductivity through the organic film. These measurements are supported by PES and NEXAFS
studies, and thus can be interpreted in terms of charge transfer and geometric structure.

8:48AM Y36.00005 Density Functional Theory of Transition Metal Phthalocyanines, NOA MAROM, LEEOR KRONIK, Weizmann Institute of Science, Israel. — Metal phthalocyanines (MPC’s) are a family of highly stable molecules that, as a molecular solid, form organic semiconductors. They have been used in a broad range of applications, e.g., light emitting diodes, solar cells, gas sensors, thin film transistors, and even as single molecule devices. Here, we present a systematic density functional theory (DFT) study of the electronic structure of selected transition metal PCs: CuPc, NiPc, CoPc, MnPc, and FePc. We critically assess the performance of several semi-local and hybrid exchange-correlation functionals for these systems, and compare the results to experimental photoemission data. For the low-spin systems CuPc, NiPc, and CoPc, we show that semi-local functionals fail qualitatively, primarily because of under- binding of localized orbitals due to self-interaction errors. For the intermediate-spin systems MnPc and FePc, we show that DFT calculations are extremely sensitive to the choice of functional and basis set with respect to the obtained electronic configuration and to symmetry breaking. However, interestingly, all simulated spectra are in good agreement with experiment despite the differences in the underlying electronic configurations.

9:00AM Y36.00006 Cascade and Accumulation of Spin at CuPc/GaAs (100) interface, HUANJUN DING, IRFAN IRFAN, YONGLI GAO, Department of Physics and Astronomy, University of Rochester, MIRKO CINCCHETTI, MARINA SANCHEZ-ALBANEDA, JAH-SUP HONG, IRFAN IRFAN, OLEKSII ANDREYEV, MICHAEL BAUER, MARTIN AESCHLIMANN, Department of Physics, University of Kaiserslautern. — We have investigated the spin dynamics in organic semiconductor, copper phthalocyanine (CuPc), with spin and time resolved two photon photoemission spectroscopy (STR-2PPE). Spin polarized electrons are generated optically from GaAs substrate, and injected into the unoccupied states of CuPc film. The apparent spin relaxation time is observed to have strong energy dependence. The spin polarization at high energy levels decreases much faster than that of the low energy levels. The experimental results are then explained by a cascade model. The calculation suggests that the spin information of the hot electrons can be well preserved during the energy relaxation process.

9:12AM Y36.00007 Electronic structure of MoO3 insertion layer at the interface between organic semiconductor and indium tin oxide (ITO), HUANJUN DING, IRFAN IRFAN, Department of Physics and Astronomy, University of Rochester, YONGLI GAO, university of rochester, FRANK SO, Department of Materials Science and Engineering, University of Florida. — We have investigated the electronic structure of the interfaces formed by inserting thin layer of MoO3 in between indium tin oxide (ITO) and different organic semiconductors, such as aluminium phthalocyanine chloride (AlPcCl) and copper phthalocyanine (CuPc), with photoemission and inverse photoemission spectroscopy (PES and IPES). The presents of MoO3 layer at the interface increases the workfunction dramatically. As a result, the organic HOMO is almost aligned with the Fermi level (EF) at the AlPcCl/MoO3 interface. For thicker AlPcCl layers, gradual band bending is observed. However, the recovery of the HOMO is incomplete for AlPcCl thickness of 200 Å, leading to a great reduction of the hole injection barrier compare to the case without MoO3. Similar situation is found in case of CuPc/MoO3, although the energy levels are almost fully recovered for CuPc film thicker than 200 Å. The energy level alignment of these interfaces will be discussed to explain the improved induced by MoO3 layer in device performance.

9:24AM Y36.00008 HPLC and Semi-Prep Scale Fractionations of Poly(3-alkyl thiophenes), SCOTT LEFEVRE, Rensselaer Polytechnic Institute, HEUNGYEOL CHOI, TAIHYUN CHANG, Pohang University of Science and Technology, CHANG RYU, Rensselaer Polytechnic Institute — Organic molecular nanofibers have been used in a broad range of applications, e.g., light emitting diodes, solar cells, gas sensors, thin film transistors, and even as single molecule devices. Here, we present a systematic density functional theory (DFT) study of the electronic structure of selected transition metal PCs: CuPc, NiPc, CoPc, MnPc, and FePc. We critically assess the performance of several semi-local and hybrid exchange-correlation functionals for these systems, and compare the results to experimental photoemission data. For the low-spin systems CuPc, NiPc, and CoPc, we show that semi-local functionals fail qualitatively, primarily because of under- binding of localized orbitals due to self-interaction errors. For the intermediate-spin systems MnPc and FePc, we show that DFT calculations are extremely sensitive to the choice of functional and basis set with respect to the obtained electronic configuration and to symmetry breaking. However, interestingly, all simulated spectra are in good agreement with experiment despite the differences in the underlying electronic configurations.

9:36AM Y36.00009 Tailored Assembly of Organic Molecular Nanofibers into Advanced Donor-Acceptor Architectures, VOLODIMYR DZUHKO, MICHAEL J. KELLEY, KENNETH D. SINGER, Case Western Reserve University. — Non-covalent self-assembly of organic molecules in organic solvents provides a multi-functional approach toward producing organic semiconducting nanostructures having versatile, well-ordered, architectures that are potentially integrable into useful electronic, optoelectronic and photonic device architectures. Aiming at molecular-scale tailoring of electron donor-acceptor blend architectures and rational engineering of their functionality for photovoltaic applications, we discuss our approach of solvent-based, electronic-field-activated integration of self-assembled donor (phthalocyanine) nanofibers into an acceptor (perylenediimide) matrix (or vice versa). We present results of our systematic spectroscopic, X-ray diffraction and scanning electron microscopy studies revealing the structure and morphology of neat fibers and fiber blends in various phases.

9:48AM Y36.00010 The substitution effect on the reorganization energy of metal free phthalocyanine, CHOONGKEUN LEE, KARL SOHLBERG, Department of Chemistry, Drexel University, Philadelphia, Pennsylvania 19104-2875. — Many discotic (disk-like) materials such as phthalocyanines are of interest for use in organic electronic devices because of their high charge mobility. The mobility of various discotic materials has been studied using the Marcus formalism. In the Marcus formalism, charge mobility is depends on two parameters, reorganization energy and coupling matrix constant.


9:48AM Y36.00010 The substitution effect on the reorganization energy of metal free phthalocyanine, CHOONGKEUN LEE, KARL SOHLBERG, Department of Chemistry, Drexel University, Philadelphia, Pennsylvania 19104-2875. — Many discotic (disk-like) materials such as phthalocyanines are of interest for use in organic electronic devices because of their high charge mobility. The mobility of various discotic materials has been studied using the Marcus formalism. In the Marcus formalism, charge mobility is depends on two parameters, reorganization energy and coupling matrix constant. Of these two parameters the reorganization energy has more influence on the charge hopping rate. A small change in reorganization energy leads to a large change of charge mobility. We have employed electronic structure methods to describe substitution effects on the reorganization energy of phthalocyanine. The substitutions on the external phenyl rings have almost no influence on reorganization energy, but the substitutions on the internal nitrogen in phthalocyanine have strong influence on reorganization energy. The detailed relation between reorganization energy and substitution will be presented.
Our recent experiments on single-molecule metal-to-ligand electron transfer (3) and single-molecule STM manipulation will also be discussed. Dynamic disorders in the dynamics. Furthermore, we have applied site-specific AFM-Raman spectroscopy on analyzing ET associated mode-specific vibrational to seconds. The fluctuation dynamics were found to be inhomogeneous from molecule to molecule and from time to time, showing significant static and at the surface of TiO$_2$.

Ensemble-averaged studies have indicated inhomogeneous and complex dynamics of interfacial ET reaction. To characterize the inhomogeniety and the complex Photochemical Sciences, Bowling Green, OH 43403 — Interfacial electron transfer dynamics is important for environmental and catalytic reactions. Extensive

The best to date discotics are built around the coronene unit and possess six fold symmetry. In the discotic phase six fold symmetric molecules stack with an average azimuthal twist of 30 deg, whereas the angle which would lead to the greatest electronic coupling and hence highest charge mobility is 60 deg. Here, a molecule with three fold symmetry and alternating hydrophilic/hydrophobic side chains is synthesized and X-ray scattering is used to prove the formation of the desired helical microstructure. Pulse radiolysis time resolved microwave conductivity measurements show that the material has indeed a very high mobility in the plastic crystalline phase, in the range of 0.1 – 0.2 cm$^2$/Vs. The physical structure of the assemblies of molecules are simulated using molecular dynamics. This, together with quantum chemical techniques, allows the computation of charge mobilities without fitting parameters. The calculations prove that mobility is still limited by structural defects and that a defect free assembly would lead to mobilities in excess of 10 cm$^2$/Vs.

1DPG is acknowledged for the financial support.

10:12AM Y36.00012 Anisotropic phases in ferromagnetic ultrathin films from multipolar interactions1, DANIEL BARCI. University of the State of Rio de Janeiro, Brazil, DANIEL STARIOLO, Federal University of Rio Grande do Sul, Brazil — We present a model to describe complex phases observed at mesoscopic scales in ultrathin magnetic films with perpendicular anisotropy. The model is based on the interaction between magnetic dipolar as well as quadrupolar moments. This model has a very rich phase diagram. In the special case of films with strong perpendicular anisotropy, a nematic phase, characterized by orientational (stripe-like) but not translational order, is predicted. The isotropic-nematic transition belongs to the Kosterlitz-Thouless type in the thermodynamic limit. However, we find that in actual experimental scales the fluctuations of the nematic order parameter are regularized by the sample size, and real orientational order, as predicted by mean field, should be observable. The transition may be characterized experimentally from measurements of the magnetic structure factor, from which the nematic order parameter is derived.

1Partially supported by the Brazilian agencies CNPq and FAPERJ.

10:24AM Y36.00013 ABSTRACT WITHDRAWN —

Friday, March 20, 2009 8:00AM - 10:36AM —

Session Y37 DCP: Mesoscopic Systems, Clusters, and Nanoscale Systems I

8:00AM Y37.00001 Single-Molecule Interfacial Electron Transfer Dynamics at Dye-Sensitized TiO$_2$ Nanoparticles. H. PETER LU, YUANMIN WANG, YUFAN HE, Bowling Green State University, Department of Chemistry, Center for Photochemical Sciences, Bowling Green, OH 43403 — Interfacial electron transfer dynamics is important for environmental and catalytic reactions. Extensive ensemble-averaged studies have indicated inhomogeneous and complex dynamics of interfacial ET reaction. To characterize the inhomogeniety and the complex mechanism, we have applied single-molecule spectroscopy and correlated AFM/STM imaging to study the Interfacial ET dynamics of dye molecules adsorbed at the surface of TiO$_2$ nanoparticles. The interfacial ET activity of individual dye molecules showed fluctuations and intermittency at time scale of milliseconds to seconds. The fluctuation dynamics were found to be inhomogeneous from molecule to molecule and from time to time, showing significant static and dynamic disorders in the dynamics. Furthermore, we have applied site-specific AFM-Raman spectroscopy on analyzing ET associated mode-specific vibrational reorganization energy barriers. Our experiments revealed site-to-site variations in the vibrational reorganization energy barriers in the interfacial ET systems. Our recent experiments on single-molecule metal-to-ligand electron transfer (3) and single-molecule STM manipulation will also be discussed.

8:12AM Y37.00002 Phase Diagram of a Model of Nanoparticles in Electrolyte Solutions. XIAOFEI LI, STEVEN LETTIERI, NATHANIEL WENTZEL, JAMES GUNTON, Lehigh University — We obtain accurate fluid-fluid coexistence curves for a recent simple model of interacting nanoparticles that includes the effects of ion-dispersion forces. It has been proposed that these ion dispersion forces provide at least a partial explanation for the Hofmeister effect [Phys. Rev. Lett., 87:168103, 2001]. We study a model of aluminum oxide nanoparticle [Colloids and Surfaces A, 319:98-102, 2008] for three different electrolyte solutions with added salt type being sodium chloride, sodium iodide and a non-polarizable salt. We observe that the fluid-fluid coexistence curves depend substantially on the identity of added salt; this provides an efficient way of tuning the phase behavior of nanoparticles. The methods we employ include finite-size scaling (FSS), multicanonical histogram reweighting and Gibbs ensemble methods. We show that, as expected, all three cases belong to the universality class. The scaling fields and critical point parameters are obtained in the thermodynamic limit of infinite system size by extrapolation of our FSS results.

8:24AM Y37.00003 Prediction of Zeolite Framework Types by a Machine Learning Approach. SHUJIANG YANG, MOHAMMED LACH-HAB, IOSIF VAISMAN, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 22030 — Zeolites are microporous crystalline materials with highly regular framework structures consisting of molecular-sized pores and channels. Characteristic framework types of zeolites are traditionally determined by the combined information of coordination sequences and vertex symbols. Here we present a machine learning model for classifying zeolite crystals according to their framework types. An eighteen-dimensional feature vector is defined including topological descriptors and physical/chemical properties of zeolite crystals [Microporous and Mesoporous Materials 117, 339 (2009)]. Trained with crystallographic data of known zeolites, the new model can predict the framework types of unknown zeolite crystals with up to 98 % accuracy. Compared with conventional methods, the machine learning model is more robust handling crystal disorder and/or crystal defects in a more effective manner. This model can be adapted for classifying and clustering other crystalline species.

1Supported by NSF grant CHE-0626111
8:36AM Y37.00044 Site-specific polarizabilities as predictors of optimal binding sites of H₂O on Naₓ clusters. LI MA, KOBLAR JACKSON, Physics Dept., Central Michigan University, Mount Pleasant, MI 48859. JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL 60439 — We have used density functional theory (DFT), in the generalized gradient approximation to study the adsorption of water molecules on sodium clusters, Naₓ for n = 7, 12, 18, and 25. These clusters span a range of sizes and surface topographies. In each case, we conduct an extensive search to identify the optimal binding site of the ad-molecule on the cluster. We analyze the results within the framework of cluster polarizability, making use of a new methodology for partitioning the cluster polarizability into atomic components (Jackson et al., J. Chem. Phys. 129, 144309 (2008)). We show that the most favorable adsorption sites are at surface atoms that have the largest atomic polarizabilities. We will compare and contrast these results with corresponding findings for the adsorption of O₂ and NH₃ molecules on Naₓ clusters.

8:48AM Y37.00055 Effect of adsorbates on the isomer stability of Ir₄ clusters. VLADAN STEVANOVIC, ITP-EPFL and IRPMA, CH-1015 Lausanne, Switzerland, ZELIKO SLJIVANCANIN, IRPMA, CH-1015 Lausanne, Switzerland, ALFONSO BALDERESCHI, ITP-EPFL and IRPMA, CH-1015 Lausanne, Switzerland and Dipartimento di Fisica Teorica, Università di Trieste, I-34014 Trieste, Italy — The relative stability of Ir₄ isomers, both in the gas phase and on MgO(100) substrate, is studied using density functional theory. The square Ir₄ is the most stable in both cases. The metastable tetrahedral isomer, which experimental data suggest as the most stable form of Ir₄ on MgO(100), is highly distorted by the strong Ir–Ir interactions. The relative stability of Ir₄ isomers is strongly altered by adsorption of a single C atom since the binding energy of the C adatom to tetrahedral and butterfly Ir₄ is much larger (~1.7 eV) than that to the square one, both in the gas-phase and on MgO(100). After carbon adsorption, the most stable structure of Ir₄ is the butterfly geometry for free clusters and the “tetrahedral” one for Ir₄/MgO(100). The C adatom binds in a bridge configuration in all cases and reduces the distortions produced by the MgO substrate. Energetics and equilibrium atomic geometries will also be discussed for the adsorption (i) one H or O atom and (ii) one CO molecule.

9:00AM Y37.00066 Control and manipulation of Au nanocatalysis: effects of metal oxide support thickness and composition. BOKWON YOON, School of Physics, Georgia Institute of Technology, CHRIS HARDING, VAHIDEH HABIBPOUR, SEBASTIAN KUNZ, ADRIAN NAM-SU FARNBACHER, UELI HEIZ, Lehrstuhl fur Physikalische Chemie, Technische Universität München, Germany, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Control and tunability of the catalytic oxidation of CO by gold clusters deposited on MgO surfaces grown on molybdenum, Mo(100), to various thicknesses, are explored through temperature programmed reaction measurements on mass selected 20-atom gold clusters and via first-principles density-functional theory calculations. Dependencies of the catalytic activities and microscopic reaction mechanisms on the thickness and stoichiometry of the MgO films, and on the dimensionalities and structures of the adsorbed gold clusters are demonstrated and elucidated. Langmuir-Hinshelwood mechanisms and reaction barriers corresponding to observed low and high temperature CO oxidation reactions are calculated and analyzed. Along with the oxidation reactions on stoichiometric ultra thin MgO films we also study reactions catalyzed by Au₅₉ nanoclusters adsorbed on relatively thick defect-poor MgO films supported on Mo, and on defect-rich thick MgO surfaces containing oxygen vacancy defects.

9:12AM Y37.00077 Role of anharmonic contributions for the elasticity of ice. MIRA TODOROVA, LARS ISMER, JÖRG NEUGEBAUER, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf — Water, one of the simplest molecules in chemistry, forms a liquid and solid phase with features essential to live and environment. Many of these can be attributed to hydrogen bonding, but that does not mean that they are fully understood. For water, there should be an easier material to understand, because its properties are somewhat understandable. Yet even the determination of basic properties as the bulk modulus and the elastic constants proves to be a challenge. Using first principles calculations we investigate the bulk properties of hexagonal ice. Our initial density-functional theory calculations (GGA-PBE level) yield values, which are much too high when compared to experiment. Even though the consideration of thermal effects within the quasi-harmonic approximation leads to a qualitative agreement between measured and calculated quantities, such as the linear expansion coefficient, ice remains much too hard. The large overestimation of the ice’s softness demonstrates the importance of anharmonic contributions, which will be shown to be crucial and lead to a dramatic reduction of the bulk modulus and the elastic constants.

9:24AM Y37.00087 An Assessment of Hubbard U Corrections on Manganese Oxide Clusters. ELISE Y. LI, Chemistry, Massachusetts Institute of Technology. DAVIDE CERESOLI, NICOLA MARZARI, DMSE, Massachusetts Institute of Technology — Conventional density-functional approaches often fall in offering an accurate description of the spin-reversed energetics in transition metal complexes, due to spurious self-interaction errors (SIE). Previous studies have shown that a self-consistent DFT + U approach [1] can accurately correct SIE in TM complexes, providing excellent agreement with high-level quantum chemistry calculations. In this work we report a systematic evaluation of DFT + U in a series of small manganese oxide clusters (MnOₓ, x=1-4) and via first-principles density-functional theory calculations. Dependencies of the catalytic activities and microscopic reaction mechanisms on the thickness and stoichiometry of the MgO films, and on the dimensionalities and structures of the adsorbed gold clusters are demonstrated and elucidated. Langmuir-Hinshelwood mechanisms and reaction barriers corresponding to observed low and high temperature CO oxidation reactions are calculated and analyzed. Along with the oxidation reactions on stoichiometric ultra thin MgO films we also study reactions catalyzed by Au₅₉ nanoclusters adsorbed on relatively thick defect-poor MgO films supported on Mo, and on defect-rich thick MgO surfaces containing oxygen vacancy defects.

9:36AM Y37.00097 ABSTRACT WITHDRAWN — 8:48AM Y37.00010 Advances in a Joint Density-Functional Theory for Electronic Systems in Contact with Liquid Water: A New Form of Density Functional for Water. JOHANNES LISCHNER, TOMAS ARIAS, Cornell University — We present a framework for studying complex electronic systems, such as biological molecules or electrochemical interfaces, that are dissolved in liquid water. The key ingredient, that renders calculations possible, is the usage of an approximate, yet accurate “classical” density-functional theory of water, while the electronic system is described by traditional Kohn-Sham theory. The electronic system (e.g. biosolite) is then coupled to the aqueous environment via molecular pseudopotentials. Here, we present a new form of “classical” density functional for water which is the first to properly account for the structure of the molecule in an exact way. We accomplish this by writing the free energy in terms of three effective potentials, one for the oxygen and one for each hydrogen atom, in which fictitious non-interacting water molecules move. In this talk, we will show that the resulting functional correctly reproduces the following properties of water: the linear and nonlinear dielectric response, the site-site correlation functions, the surface tension, the bulk modulus of the liquid and its variation with pressure, the density of the liquid and the vapor phases, and their coexistence.

10:00AM Y37.00011 The AM05 density functional applied to the water molecule, dimer, and bulk liquid. ANN E. MATTSOHN, THOMAS R. MATTSOHN, Sandia National Labs — We show that the AM05 exchange-correlation density functional (Armiento and Mattsson, Phys. Rev. B 72, 085108 (2005)) yields a H₂O dimer binding energy of 4.9 kcal/mol. The result is thus within 0.15 kcal/mol of CCSD(T) level theory (5.02 ± 0.05 kcal/mol). We compare the AM05 results with those of five other functionals: LDA, PBE, PBEsol, RPBE, and BLYP. For liquid water, AM05 yields an O–O pair correlation function that is more structured than the ones of PBE and BLYP, which, in turn, are more structured than the one of RPBE. However, LDA and PBEsol yields more structured water than AM05. We confirm that accuracy in the water dimer binding energy is not a strong indicator for the fidelity of the resulting structure of liquid water. We will also report on the performance of AM05 for other systems and discuss the sub-system functional scheme used in the construction of AM05. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
10:12AM Y37.00012 Heat capacities of aluminum clusters . ANNE STARACE, BAOPENG CAO, OSCAR JUDD, MARTIN JARROLD, Indiana University–Bloomington — Clusters of certain elements are known to undergo phase transitions from solid-like to liquid-like states. Aluminum clusters have emerged as a model system for metal cluster phase transitions [1]. We report here the measurement of heat capacities of cationic clusters containing 84 to 127 Al atoms using a multi-collision induced dissociation mass spectrometry method [2]. We find two major changes in the heat capacities with increasing cluster size: (1) the fluctuations in the temperature of the phase transition vary more smoothly and (2) the peaks in heat capacity become sharper. Furthermore, we have found a range of cluster sizes (115-117 atoms) that contain two distinct peaks, separated by baseline, in their heat capacities. The origin of the extra peaks in the heat capacity, which is suspected to be due either to a pre-melt transition or to a solid-to-solid transition prior to the melting transition, will be further investigated by means of annealing experiments. The current work extends prior work on singly charged Al cluster cations having 16-83 atoms [2, 3]. [1] Breux, G. A.; Neal, C. M.; Cao, B.; Jarrold, M. F. Physical Review Letters 2005, 94. [2] Neal, C. M.; Starace, A. K.; Jarrold, M. F. Journal of the American Society for Mass Spectrometry 2007, 18, 74-81. [3] Neal, C. M.; Starace, A. K.; Jarrold, M. F. Physical Review B 2007, 76. [4] This work is supported by NSF.

10:24AM Y37.00013 From Atomic Clusters towards Nano-Materials with Controlled properties1 . S.N. KHANNA, M.C. QIAN, A.C. REBER, J.U. REVELES, R. ROBLES, P.A. CLAYBORNE, S.V. ONG, K. CASALENUOVO, Virginia Commonwealth University, A.W. CASTLEMAN JR., A. SEN, P.W. WEISS, H. SAAVEDRA, A. UGRINOV, N. CHAKI, Pennsylvania State University — One pathway towards the synthesis of nanomaterials with controllable properties is to assemble solids using chosen clusters as the building blocks. The talk will outline a new protocol that enables synthesis of nanomaterials from clusters and highlight how the character of the cluster emerges in the assembled material. Through studies on assemblies involving polyvalent anions As7–, As5–, and alkali based cations, we will show how the studies can provide novel ways of controlling the bandgap through energy level of the countercation and the degree of charge transfer. The theoretical predictions will be compared with experimental findings.

The authors are grateful to the Army Research Office for supporting this work through a MURI grant (Grant # W911NF-06-1-0280).

Friday, March 20, 2009 8:00AM - 11:00AM –
Session Y38 DCP: Surfaces, Interfaces, and Colloids I 410

8:00AM Y38.00001 Aqueous Solutions on Silica Surfaces: Structure and Dynamics from Simulations1 . ALBERTO STRIOLO, DIMITRIOS ARGYRIS, NAGA RAJESH TUMMALA, University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING AT OU TEAM — Our group is interested in understanding the properties of aqueous electrolyte solutions at interfaces. The fundamental questions we seek to answer include: (A) how does a solid structure perturb interfacial water? (B) How far from the solid does this perturbation persist? (C) What is the rate of water reorientation and exchange in the perturbed layer? (D) What happens in the presence of simple electrolytes? To address such topics we implemented atomistic molecular dynamics simulations. Recent results for water and simple electrolytes near silicon dioxide surfaces of various degrees of hydroxylation will be presented. The data suggest the formation of a layered aqueous structure near the interface. The density profile of interfacial water seems to dictate the density profiles of aqueous solutions containing NaCl, CaCl2, CsCl, and SrCl2 near the solid surfaces. These results suggest that ion-ion and ion-water correlations are extremely important factors that should be considered when it is desired to predict the distribution of electrolytes near a charged surface. Our results will benefit a number of practical applications including water desalination, exploitation of the oil shale in the Green River Basin, nuclear waste sites remediation, and design of nanofluidic devices.

1Department of Energy

8:12AM Y38.00002 Formation of Organic Peroxides and Ethers at Post-Discharge Plasma Plume-Liquid Interfaces . MILAN BEGLJARBEKOV, STEVEN KOTOWICH, VLADIMIR TARNOVSKY, Stevens Institute of Technology — A direct current (DC) micro-hollow cathode plasma source operating in a mixed glow-streamer regime was used to generate an atmospheric pressure N2 plasma. The post-discharge plume / afterglow was interfaced with a target liquid-phase solution, and caused a change in the chemistry of the target solution. In the present work we study the interaction of an N2 plume with a mixture of 2-methyl-1-propanol and hexane, which results in the formation of organic peroxides and ethers at the plume-liquid interface. The presence of the peroxide and ether functional groups is established by 1H-NMR, FTIR, and Raman spectra of the reaction products. Fast Atom Bombardment (FAB) mass spectrometry is also used to further characterize the reaction products.

8:24AM Y38.00003 Deducing 2D Crystal Structure at the Solid/Liquid Interface with Atomic Resolution by Combined STM and SFG Study . ARTHUR MCCLELLAND, University of Michigan, Applied Physics Program, SEOKHOON AHN, ADAM J. MATZGER, ZHAN CHEN, University of Michigan, Chemistry Department — Supplemented by computed models, Scanning Tunneling Microscopy (STM) can provide detailed structural information of 2D crystals formed at the liquid/solid interface with atomic resolution. However, some structural information such as functional group orientations in such 2D crystals needs to be tested experimentally to ensure the accuracy of the deduced structures. Due to the limited sensitivity, many other experimental techniques such as Raman and infrared spectroscopy have not been allowed to provide such structural information of 2D crystals. Here we showed that Sum Frequency Generation Vibrational Spectroscopy (SFG) can measure average orientation of functional groups in such 2D crystals, or physisorbed monolayers, providing key experimental data to aid in the modeling and interpretation of the STM images. The usefulness of combining these two techniques is demonstrated with a phthalate diesters monolayer formed at the 1-phenyloctane/ highly oriented pyrolytic graphite (HOPG) interface. The spatial orientation of the ester C=O of the monolayer was successfully determined using SFG.

8:36AM Y38.00004 Curved space crystallography at an oil-water interface . WILLIAM IRVINE, STEFANO SACANNA, YAEL ROICHMAN, ANDREW HOLLINGSWORTH, MARK ELSESSER, Center for Soft Matter Research, New York University, MARK BOWICK, Physics Department, Syracuse University, DAVID GRIER, PAUL CHAIKIN, Center for Soft Matter Research, New York University — We study two-dimensional crystallography on a curved oil-water interface. Charged hydrophobic (PMMA) colloids in an oil phase (cyclohexyl bromide) are attracted, without wetting, by image charge effects to an oil-water interface. The micron size spheres form a monolayer on the interface and interact via screened coulomb interactions to form a crystalline lattice. We create a curved oil-water interface by controlling wetting conditions between a water droplet and a substrate or support, to produce interfaces of both constant and varying gaussian curvature with boundary. We simultaneously image and manipulate the full crystal on the curved surface using a setup capable of simultaneous holographic optical tweezing and confocal imaging. We study the resulting dynamics of topological defects.
8:48AM Y38.00005 On the nanometer Gold projectile - surface interaction in SIMS experiments. FRANCISCO A. FERNANDEZ-LIMA, VERONICA PINNICK, MICHAEL ELLER, STANISLAV VERKHOTUROV, EMILLE SCHWEIKERT, Texas A&M University — In an effort to increase the secondary molecular ion signal under ion bombardment, a series of cluster sources have been developed with sputtering yields that deviate from the linear cascade prediction due to the collective cluster beam - surface interaction. In the present talk, the variation of the massive gold \( \text{Au}_{n}^{+} \) projectile size (n=1-400) and velocity on the interaction volume and number of desorbed/sputtered particles per impact will be discussed for alkali halide targets. As the projectile size increases, a larger number of cluster ions is observed, where the secondary ion yield can be describe as a decreasing exponential function of the cluster size. Theoretical ab initio calculations show that the relative MS abundances are related to the cluster structure stabilities, defined by a “fine” ratio of short and long range interactions between the cluster counterparts. Angular distribution measurements of the secondary ions suggest that under keV bombardment emission normal to the target surface is favored, independent of the cluster ion size. Applications of the massive gold \( \text{Au}_{n}^{+} \) projectiles as nanometric imaging probes (< 10^4 nm²) will be presented.

9:00AM Y38.00006 Binding energy of adsorbates on a noble-metal surface: Exchange and correlation effects. MICHAEL ROHLFING, University of Osnabrueck, THOMAS BREDOW, University of Bonn — We discuss the physisorption of atoms (xenon) and molecules (PTCDA) to a noble-metal surface (silver) within a first-principles approach, focusing on the adsorption energy as a function of distance. Instead of density-functional theory (which fails to describe physisorption) we employ a combination of exact exchange and correlation energies, which we evaluate within the adiabatic-connection fluctuation-dissipation theorem. Correlation accounts for non-local dispersion energy, which is crucial in the present cases. At large distance Z from the surface the correlation causes van der Waals attraction with a characteristic \(-C_{6}/(Z-Z_{0})^{6}\) asymptotic form. At closer distance the attraction deviates from the asymptotic form and, in combination with the retractive exchange-correlation energy, yields an equilibrium bond for xenon on and of PTCDA on the Ag(111) surface in close agreement with experiment.

9:12AM Y38.00007 Bonding of adenine on Cu(110). GEOFFREY STENUIT, CNR-INFM DEMOCRITOS Theory@Elettra Group, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy, OKSANA PLEKAN, VITALY FYEYER, KEVIN PRINCE, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy, PAOLO UMARI, CIN-IRN-M DEMOCRITOS Theory@Elettra Group, Sincrotrone Trieste, in Area Science Park, I-34012 Basovizza (Trieste), Italy — We present a density functional study of the adsorption of adenine molecules on the Cu(110) surface. In agreement with experimental core level photoemission and x-ray absorption data, our calculations predict the existence of two phases: a parallel one at low coverage and a perpendicular one at high coverage. These findings resolve contradictions between calculated geometries and published vibrational spectra, and illustrate the complexity of the interaction between a relatively simple bio-molecule and a metal.

9:24AM Y38.00008 ABSTRACT WITHDRAWN —

9:36AM Y38.00009 Two-photon photoemission spectroscopy of thiophene/Au(111).1, JING ZHOU, Chemistry Department, Stony Brook University, Stony Brook, NY 11794, NICHOLAS CAMILLONE, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, MICHAEL WHITE, Chemistry Department, Stony Brook University & Chemistry Department, Brookhaven National Laboratory — The electronic structure of thiophene adsorbed on Au(111) is investigated by two-photon photoemission (2PPE) spectroscopy and density functional theory (DFT) calculation. The adsorption of thiophene lowers the work function from 5.50 eV for clean Au(111) to 4.62 eV for Au(111) exposed to 4.0 L thiophene, due to the electron donation from the thiophene to the substrate. With thiophene adsorbed on Au(111), a localized \( \sigma^* \) state forms with increasing thiophene exposure on Au(111). This \( \sigma^* \) state is attributed to the \( \pi^* \) antibonding orbital of a Au-S bond and is evidence of an orientational phase transition of thiophene adsorbed. Preliminary 2PPE results will also be presented for aromatic molecules bound to the Au surface via sulfur or other functional goups (e.g., isocyanide).

1 This work is supported by the US Department of Energy, Office of Basic Energy Science, Division of chemical sciences under contract DE-AC02-98CH10886.

9:48AM Y38.00010 Interfacial Structure imaging of Pentacene/Si(111) by model- independent method. SONGTAO WO, HUA ZHOU, RANDALL HEADRICK, University of Vermont, ALEXANDER KAZIMIROV, Cornell High Energy Synchrotron Source, CORNHILL HIGH ENERGY SYNCHROTRON SOURCE TEAM — Synchrontron x-ray reflectivity is utilized to study the Pentacene/Si(111) interfacial structure in the direction normal to the surface. Model-independent algorithm is used to analyze the reflectivity data to extract the electron density profile. It indicates two partially ordered layers along the interfacial normal with thickness ~0.6 nm and an interfacial water layer ~0.9 nm as we reported in our previous work. A pentacene monolayer ~1.6 nm can also be revealed.

10:00AM Y38.00011 Optical Trapping of Colloidal Nanoparticles by a Weakly Focused Laser Beam. CHUN-YU LIN, HSIA-YU LIN, Lehigh University, SHEAN-JEN CHEN, STEVEN M.T. WEI, H.D. OU-YANG, Lehigh University — We present an analysis of the behavior of an ensemble of colloidal nanoparticles in the focal region of a weakly focused laser beam. Using a mechanical balance of the laser radiation pressure that causes particle migration into the light field and the osmotic pressure of these particles opposing migration, we propose a new method for quantifying the optical trapping potential of individual particles by measuring the increase of the particle concentration as a function of the laser intensity. We find comparable results for the optical trapping potential from this method with values obtained by single particle trapping methods, indicating that radiation-induced particle convection from a weakly focused laser beam does not affect the steady state distribution of the particles in the light field.

10:12AM Y38.00012 Colloidal Crosstalk: Brownian Diffusion of Hydrodynamically Coupled Colloids. STEPHEN ANTHONY, University of Illinois, MINSU KIM, UC San Diego, STEVE GRANICK, University of Illinois — Except at dilute concentrations, the Stokes-Einstein Equation inadequately describes the thermal motion of colloids, due to hydrodynamic interactions between nearby particles. Using single-particle tracking, the rotational and translational motion of hydrodynamically interacting colloids is observed, and deviations from the Stokes-Einstein Equation are readily apparent. The thermal motion of nearby colloids is found to couple in a non-additive fashion, with increasing degrees of non-linearity as particle separation decreases. Similar coupling is observed for colloids near surfaces.

10:24AM Y38.00013 Depletion-Driven Selective Optical Trapping in Nanoparticle Suspensions. YI HU, JOSEPH JUNIO, H.D. OU-YANG, Lehigh University — We report results of an optical trapping study that demonstrates the effects of size-asymmetric particles in suspension have on optical trapping efficiency. Using a model colloid system with selective fluorescent dying and particle sizing, we show that the trapping efficiency of nanoparticles can be effectively tuned by adding different sized particles, promoting the use of optical trapping for particle sorting. A variable power IR laser coupled into a high NA objective was used for trapping. For particle detection, we used a 532nm excitation laser aligned to be parfocal with the IR trapping beam through the same objective lens. Fluorescent signals emanating from the focal region common to both beams was band-passed to a pinhole set to be conjugate to the focal region for confocal detection. In a system composed of 160nm and 63nm particles we demonstrated the synergistic effect of size mixing. Experimental results are also shown for fluorescent particles being driven out of the region by size selective trapping of undesired 160nm particles.
10:48AM Y38.00015 Determination of Charge Interactions of Nanoparticles by Optical Trapping, JOSEPH JUNIO, H.D. OU-YANG, Lehigh University — We report an experimental study of interactions in colloidal nanoparticles through optical trapping. Using an optical trap with a size much larger than the trapped particles, we were able to create an optical bottle to confine and concentrate the nanoparticles. We measured the highly focused light-induced particle density fluctuation with confocal fluorescent detection. A theory based on a balance between the optical trapping radiation pressure and the osmotic pressure has been developed to calculate the isothermal osmotic compressibility from the forced density fluctuation. The measured osmotic compressibilities of colloidal crystals are then used to determine the surface charge density of the colloidal particle(1). Comparison of the experimentally determined charge density is compared to that determined by zeta potential measurements. (1)S. Alexander, P. M. Chaikin, P. Grant, G. J. Morales, and P. Pincus, D. Hone, Charge renormalization, osmotic pressure, and bulk modulus of colloidal crystals: Theory, J. Chem. Phys. 80, 5776 (1984).

Friday, March 20, 2009 8:00AM - 11:00AM
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8:00AM Y39.00001 The Molecular Splash Test: when applied physics help stroke patients, CEDRIC HURTH, LENA VAN NIMWEGEN, DEEPTHI JAMPALA, Applied Nanobioscience, Biodesign Institute, KRIS VIJAY, Scottsdale Clinical Research Institute, FREDERICK ZEHNHAUSERN, Applied Nanobioscience, Biodesign Institute — The Molecular Splash Test (MST) stems from recent observations of a solid sphere producing a splash when impacting a liquid (Bocquet et al. 2007, Nature Physics, 3, 180). We have developed the experimental setup incorporating a high-speed camera operated at 8,000 frames/s to perform biologically-relevant experiments, e.g. rheology studies from the impact of a native glass bead and molecular recognition tests when the impacting bead is functionalized with biomarkers. We present preliminary results with millimeter-sized glass beads impacting water mixtures of increasing glycerol content, i.e. increasing viscosities, as well as biotin-modified glass beads impacting avidin solutions (0.1 – 1 mg/mL). The viscosity increase of a human blood sample containing hirudin, once hirudinase II is added to re-induce coagulation, is monitored over time to assess the ability of MST to function on samples of medical interest. The beads can then be derivatized with an antibody for detection of C-reactive protein in blood serum.

8:12AM Y39.00002 Surfaced-Enhanced Raman Scattering of λ-DNA1, DIANE ALVAREZ, JIANDI ZHANG, Louisiana State University, Baton Rouge, LA 70803, HONG WEI, HONGXING XU, Institute of Physics, CAS, Beijing, 100080, China — The ability to engineer metal particles at the nanoscale in which plasmons can be excited, directed, and manipulated has led to the rapid development of the field of “plasmonics”. Here we demonstrate that the Raman scattering of λ-DNA molecules with colloidal silver nanoparticles is drastically enhanced by surface plasmon excitations. Colloidal silver nanoparticles (~90 nm size) were assembled onto DNA molecules using the molecular combing method. Surface-enhanced Raman scattering (SERS) spectra were obtained and compared for different solution concentrations of the DNA/Ag system. It is evident that the SERS peaks were shifted to a lower or higher wavenumber, depending on the concentration of the solution. These different shifts of Raman frequencies may indicate that the different stretching states of DNA molecules in different concentrations probably influence the Raman frequencies. It is speculated that the coiling states of DNA molecules might be different in different concentrations, thus making it a promising method for the study of DNA functionalities and DNA-nanoparticle interactions.

1Supported by China NSF 10625418 & 90406024, MOST Grant No. 2006DFB02020, and US NSF CIEH-0415421.

8:24AM Y39.00003 Sub-cellular structure studied by combined atomic force-fluorescence microscopy1, ANDREEA TRACHE, Texas A&M Health Science Center — A novel experimental technique that integrates atomic force microscopy (AFM) with fluorescence imaging was used to study the role of extracellular matrix proteins in cellular organization. To understand the mechanism by which living cells sense mechanical forces, and how they respond and adapt to their environment, we developed a new technology able to investigate cellular behavior at sub-cellular level that integrates an AFM with total internal reflection fluorescence (TIRF) microscopy and fast-spinning disk (FSD) confocal microscopy. Live smooth muscle cells exhibited differences in focal adhesions and actin pattern depending on the extracellular matrix used for substrate coating. Data obtained by using the AFM-optical imaging integrated technique offer novel quantitative information that allows understanding the fundamental processes of cellular reorganization in response to extracellular matrix modulation. The integrated microscope presented here is broadly applicable across a wide range of molecular dynamics studies in any adherent live cells.

1Supported by NSF CAREER and AHA-National SDG to AT.

8:36AM Y39.00004 Expanding the applicability of multi-photon fluorescence recovery after photobleaching in vivo by incorporating convective flow into the recovery model1, KELLEY SULLIVAN, University of Rochester Department of Physics and Astronomy, WILLIAM SIPPRELL, University of Rochester Department of Biomedical Engineering, EDWARD BROWN, JR., Manhattan College Department of Physics, EDWARD BROWN, III, University of Rochester Department of Biomedical Engineering — Multi-photon fluorescence recovery after photobleaching is a well-established microscopy technique used to study diffusion, with expanding applications in vivo. We present a new model of fluorescence recovery that explicitly includes the effect of convective flows within a system, thereby improving the efficacy of the technique in vivo, where convective flows are omnipresent. We test this “flow” model through both simulations and in vitro experimentation, and demonstrate the effectiveness of the new model in vivo. Our results show that the flow model significantly improves the capabilities of multi-photon fluorescence recovery after photobleaching in vivo, by enabling an accurate determination of the diffusion coefficient, even when significant flows are present.

1This work was funded by a Department of Defense Era of Hope Scholar Award (W81XWH-05-1-0396) and a Pew Scholar in the Biomedical Sciences Award to Edward Brown III.
8:48 AM Y39.00005 Electrophoretic Migration of Branched DNA in Polymer Solutions. HENRY LAU, LYNDEEN ARCHER, School of Chemical and Biomolecular Engineering, Cornell University — The electrophoretic migration of large, star-branched DNA molecules has previously been studied in both neutral polymer solutions and gels, and the results have provided insight into the local interactions between the analytes and the sieving matrix during electrophoresis (Electrophoresis, 2006, 27, 3128). This talk focuses on using rigid-rod DNA molecules of complex shapes as model analytes in studying the effects of analyte architecture on mobility in polymer solutions. Electrophoresis of a series of Y-shaped DNA molecules that mimic the shapes of antibodies, was performed in polymer solutions above the overlap concentration and at electric fields up to 300V/cm. The location of the branch point as well as the arm sizes are varied in order to examine their influence on mobility. Our results point to novel, topology-based fractionation strategies for separating biological molecules using capillary electrophoresis with polymer sieving media.

9:00 AM Y39.00006 Time-resolved dielectric spectroscopy of protein aggregation performed on model system of hen lysozyme and beta-lactoglobulin. BRIAN MAZZEO, Brigham Young University, ANDREW FLEWITT, University of Cambridge — Time-resolved dielectric spectroscopy measurements of solutions containing hen lysozyme and beta-lactoglobulin reveal changes in electrical configuration and hydrodynamic parameters during their interaction. These measurements were performed in a temperature-controlled dielectric cell connected to an HP4194A impedance analyzer. The protein titrations were performed by sequential additions of reacting proteins. Differential spectra reveal the electrical contributions by each species. The computer-controlled measurements and relevant post-processing of the obtained spectra allow quantitative extraction of reaction parameters. This is demonstrated for a model system of proteins consisting of hen lysozyme and beta-lactoglobulin. Reorientation time constants, dielectric increments, and relaxation spread parameters are plotted against time and indicate binding processes. The technique is demonstrated to be a useful analytical tool for monitoring reactions in biological and colloidal systems.

9:12 AM Y39.00007 “Shooting Bead” Method with Filament Energy Loss Consideration for Finding the Flexural Rigidity of the Rodelike Biological Filaments. ABDORREZA SAMARBKHSH, JACK TUSZYNSKI1. Department of Physics, University of Alberta, Edmonton, Canada — Flexural rigidity is one of the important characteristics of flexible polymers including biological filaments. For elastic deformation it is analogous to the spring constant in the Hook’s law for bending. In this work we propose a new method for experimentally evaluating the cantilever stiffness and flexural rigidity of semiflexible rodlike biological filaments based on the measurement of just two distances. The method is based on applying a force normal to the filament with a microsphere bead trapped in the laser tweezer followed by its sudden release. Through two simple measurements of the initial and final position of the bead, the cantilever stiffness and flexural rigidity of the filament can be found from the formula that has been provided. In the second part, the effect of filament radius has been taken into account and a new formula with filament energy loss consideration, for flexural rigidity and the cantilever stiffness has been found.

9:24 AM Y39.00008 Electrostatic Force Microscopy Identification of Different Peptide Structures, CASPER HYTTTEL CLAUSEN, DTU Nanotech — In this work electrostatic force microscopy (EFM) was used to distinguish between different dipeptides tubes, silver filled peptides, spheres and silver wires, all the samples were placed on pre fabricated SiO2 surfaces with a backgate under ambient conditions. The EFM method used for the experiments was force gradient signal, which uses a dual scan approach in order to minimize the atomic force interactions. The investigation shows that it is possible to distinguish between the three types of structures. Further an agreement between the detected signal and the structure of the hollow peptide was demonstrated. These measurements only show qualitative agreement with the mathematical expressing for the peptide tubes. Further during EFM mapping of the silver filled peptide structures showed a changing effect between the tip and the sample. Investigations of this effect were carried out in order to get a better understanding of the physical properties of the peptide structures.

9:36 AM Y39.00009 Specific Detection of Vascular Endothelial Growth Factor Using Microcantilever Resonators. JASON FRANCIS, Dept. of Physics, West Virginia University, STEPHANIE ARCHER, LISA HOLLAND, Dept. of Chemistry, West Virginia University, DAVID LEDERMAN, Dept. of Physics, West Virginia University — We demonstrate the specific detection of vascular endothelial growth factor, a protein indicated in tumor angiogenesis, using resonant frequency shifts in microcantilevers due to mass loading, avoiding the need to use tagged antibodies and multiple reagents as is needed with enzyme linked immunosorbent assays (ELISA). Cantilever surfaces were functionalized using F(ab')2 fragments linked to gold surfaces via their native thiol groups, eliminating the need for complex linking processes. The cantilever surfaces were then passivated with bovine serum albumin to minimize shifts due to nonspecific binding. This technique allows the detection of pg/ml-level concentrations of analyte.

1This work is supported by National Science Foundation (grant EPS-0314742) and the WVNano Initiative at West Virginia University.

9:48 AM Y39.00010 Positioning and guidance of neurons on Au by directed assembly of proteins using Atomic Force Microscopy. CRISTIAN STAII, Department of Physics, University of Wisconsin, Madison. CHRISS VIESSELMANN, JASON BALLWEG, Department of Anatomy, UW-Madison, JUSTIN WILLIAMS, Department of Biomedical Engineering, UW-Madison, ERIK DENT, Department of Anatomy, UW-Madison, SUSAN COPPERSMITH, MARK ERIKSSON, Department of Physics, UW-Madison — The specific interactions between neurons and guidance factors as well as the mechanism of axonal navigation toward a target in the developing brain are not well understood. To address this problem we present a new approach for controlling the adhesion, growth and interconnectivity of cortical neurons on Au surfaces. Specifically, we use AFM nanolithography to immobilize extracellular matrix proteins at well-defined locations on Au surfaces, and show that these protein patterns can confine neuronal cells and control their growth and interconnectivity. We will compare this method with other nanofabrication techniques and discuss its main advantages: 1) the procedure is carried out in aqueous solutions, so that the proteins retain their bioactivity, 2) a high degree of control over location and shape of the protein patterns can be achieved, and 3) the minimum protein feature size can be as small as 50nm.

1work supported by ICAM and UW-Madison NSEC

10:00 AM Y39.00011 Determination of Frank-Oseen parameters in collagen using polarization modulated second harmonic signal. CLAYTON BRATTON, University of California, Davis - Physics, KAREN REISER, University of California, Davis - Neurosurgery, ANDRE KNOESEN, DIEGO YANKELEVICH, MINGSHI WANG, University of California, Davis - Electrical and Computer Engineering, ISRAEL ROCHA - MENDOZA, Cardiff University, Cardiff, Wales - Cardiff School of Biosciences — A method is presented for determining the Frank-Oseen parameters for the elastic modulus of collagen based on analysis of polarization-modulated second harmonic signal (PM-SHG). The liquid crystal structure of collagen and its associated order parameter, the director field, were characterized in samples of tendon and annulus fibrosus. Deformation of the director field caused by controlled stress loading or heating was assessed. Three distinct curvature strains—splay, twist, and bend—were determined, using the PM-SHG data. This optical technique permits highly localized determination of the three major elastic deformations.
10:12AM Y39.00012 Direct measurement of the non-conservative force field generated by optical tweezers, PINYU WU, RONGXIN HUANG, University of Texas - Austin, Austin, TX USA, CHRISTIAN TISCHER, ALEXANDR JONAS, ERNST-LUDWIG FLORIN, University of Texas - Austin, Austin, TX USA — Optical tweezers have been widely used in soft condensed matter physics and biophysics to measure forces in molecular processes on the single molecule level. The usual assumption is that the force applied to a particle confined with the tweezers is directly proportional to the displacement of the particle from the trapping center, which would imply that the force field of the tweezers is conservative. However, the Gaussian beam model indicates that this force field is actually non-conservative, yet no experiments have measured this effect. We developed a new experimental method that can directly measure the force field with femtonewton precision without assuming its conservative character. We successfully obtained the 3-D force field for an optically trapped Rayleigh particle with 10 nm resolution by analyzing its Brownian motion. We found a non-conservative contribution that increases as the trapped particle moves away from the optical axis. In the light of this finding, optical trapping experiments that assumed a conservative force field may need careful reevaluation.

10:24AM Y39.00013 SERS-Active Nanoinjector for Intracellular Spectroscopy, ELINA VITOL, Drexel University, ZULFIYA ORYNBAYEVA, MICHAEL BOUCHARD, JANE AZIZKHAN-CLIFFORD, GARY FRIEDMAN, YURY GOGOTSI, KECK INSTITUTE FOR ATTOFLUIDIC NANOTUBE-BASED PROBES TEAM — We developed a multifunctional nanopipette which allows simultaneous cell injection and intracellular surface-enhanced Raman spectroscopy (SERS) analysis. SERS spectra contain the characteristic frequencies of molecular bond vibrations. This is a unique method for studying cell biochemistry and physiology on a single organelle level. Unlike the fluorescence spectroscopy, it does not require any specific staining. The principle of SERS is based on very large electromagnetic field enhancement localized around a nano-rough metallic surface. Gold colloids are widely used SERS substrates. Previously, the colloidal nanoparticles were introduced into a cell by the mechanism of endocytosis. The disadvantage of this method is the uncontrollable aggregation and distribution of gold nanoparticles inside a cell which causes a significant uncertainty in the origin of the acquired data. At the same time, the nanopipette uptake is irreversible. We present a SERS-active nanoinjector, coated with gold nanoparticles, which enables selective signal acquisition from any point-of-interest inside a cell. The nanoinjector provides a highly localized SERS signal with sub-nanometer resolution in real time.

10:36AM Y39.00014 Evaluating Epithelial Mechanics with Laser Hole-drilling1, M. SHANE HUTSON, DAVID N. MASHBURN, XIAOYAN MA, HOLLEY E. LYNCH, Dept of Physics & Astronomy, Vanderbilt University — During the development of an organism, sheets of epithelial cells expand, contract and bend due to intra- and intercellular forces. We have previously developed laser hole-drilling as a technique to probe such epithelial mechanics — with a focus on the ms-to-s dynamic recoll of single, directly adjacent cell edges. Here we extend the analysis to consider ablation-induced deformations for the entire field of surrounding cells. We treat each epithelium as a homogeneous, linearly elastic, thin sheet. This simplification provides analytical solutions for the expected strain relaxation after hole-drilling (under either plane stress or plane strain). We have developed routines that use these analytic mappings (plus potential rigid body motions) to warp and match pre- and post-drilling images. These mappings account for the majority of the observed deformations and allow one to estimate the epithelium’s Poisson ratio and pre-drilling average strain tensor (which yields the anisotropy and direction of principle stress/strain). The unaccounted, residual displacements provide clues to how each epithelium deviates from a homogeneous sheet.

1Supported by NSF (I0B-0545679) and HFSP (RGP0021/2007C).

10:48AM Y39.00015 Top-Down Fabricated Silicon Nanochannel Field-Effect Transistors for Biosensing Applications, YU CHEN, XIHUA WANG, SHYAMSUNDER ERRAMILLI, PRITIRAJ MOHANTY, Physics department of Boston University, NANO LAB OF BU TEAM — Silicon nanochannel field-effect transistors have great promise for biomolecular sensing. The sensitivity is enhanced at the nanoscale due to the large surface-to-volume ratio. Specificity is achieved by functionalizing the devices with selected antibodies or complimentary target molecules. These devices are important as building blocks for high density bioanoelectronics. Top-down fabrication of these devices is compatible with advanced microfabrication processes. We show top-down fabricated silicon nanochannel devices with 3-dimensional relief can serve as a platform for biosensing applications. Three sides of the silicon nanowire are covered with a thin Al2O3 layer using Atomic Layer Deposition to form an insulating layer. When the surface is modified for binding to specific biomarkers, the device conductance change can be used to detect binding events through a field effect. Applications include building immunosensors to detect the breast cancer antigen 15-3 and other protein biomarkers, and constructing enzyme-based sensors to detect metabolites like glucose and urea.

Friday, March 20, 2009 8:00AM - 10:48AM –
Session Y40 DBP: Physiological and Medical Physics 412

8:00AM Y40.00001 Biophysical investigation of the apoptotic force1, YUSUKE TOYAMA, XOMALIN PERALTA, Duke University, Physics Department, ADRIENNE WELLS, DANIEL KIEHART, Duke University, Department of Biology, GLENN EDWARDS, Duke University, Physics Department — Understanding tissue dynamics during development requires knowledge of how cells produce and respond to forces. We have experimentally shown that apoptosis (programmed cell death, which remodels tissue by eliminating cells) also contributes a significant tissue force that promotes cell sheet fusion during dorsal closure in Drosophila development [Science, 321, 1683 (2008)]. By genetically suppressing (enhancing) apoptosis, we slow (increase) the rate of dorsal closure. These changes correlate with the forces produced by the amniotosa tissue and the rate of seam formation (zipping) for two advancing sheets of lateral epidermis. This apoptotic force is used to drive cell sheet movements during development, a role not classically attributed to apoptosis.1 This research has been supported by the NIH (GM33830).

8:12AM Y40.00002 Reorganization of neuronal circuits in growing visual cortex, WOLFGANG KEIL, MPIDS Goettingen, SIGRID LOEWEL, University Jena, FRED WOLF, MPIDS Goettingen, MATTHIAS KASCHUBE, Princeton University — The dynamics of reorganization of large cortical circuits is rooted in plasticity of individual synapses, but the rules governing the collective behavior of large networks of neurons are only poorly understood. The postnatal brain growth partly evoked by extensive formation of new synaptic connections may expose cortical areas to a ‘natural perturbation’ sufficiently strong to observe signatures of large scale reorganization. Quantifying large sets of imaging data from juvenile cat visual cortex, we observed a novel mode of reorganization of domains that prefer inputs from one eye or the other. Our theoretical analysis shows that this mode can be explained quantitatively by the so called Zigzag instability, a dynamical reorganization, well-known in the field of pattern formation in physics, by which 2D isotropic sheets of lateral epidermis. This apoptotic force is used to drive cell sheet movements during development, a role not classically attributed to apoptosis.

This research has been supported by the NIH (GM33830).
8:24 AM Y40.00003 Epithelial oscillations enhance signal detection in a peripheral sensory system. ALEXANDER NEUMAN, Ohio University, TATIANA ENGEL, Yale University School of Medicine, DAVID RUSSELL, BRIAN HELBIG, Ohio University, LUTZ SCHIMANSKY-GEIER, Humboldt University at Berlin — Rhythmic spontaneous activity was observed in various peripheral sensory systems. Many sensory receptors have a specific structure where detector cells in a sensory epithelium excite primary afferent neurons. We explore how stochastic oscillations of epithelial cells affect the ability of peripheral receptors to detect weak stimuli. We use a simple analytically tractable model to contrast signal detection in two situations: (i) when epithelial oscillations are coherent, and (ii) when the coherence of epithelial oscillations is destroyed. We show that coherent epithelial oscillations decrease the variability of neuronal firing, and thus to enhance discriminability of weak signals. Model predictions are supported by the analysis of experimental data from the electoreceptors of paddlefish.

8:36 AM Y40.00004 Sound Localization in Lizards: Functioning of a Pressure-Gradient Receiver. J. LEO VAN HEMMEN, Physik Department, TU Muenchen — Because of their small interaural distance, lizards as well as some other animals have developed a special hearing mechanism, the “pressure-gradient receiver.” The lizard peripheral auditory system differs from the mammalian one by a coupling of the two eardrums through the internal mouth cavity. We present a three-dimensional analytical model of the pressure-gradient receiver. The central aspect of the coupling of the membranes through the mouth cavity is realized by means of the boundary conditions. Moreover, the lizard’s middle ear, a simple lever construction called columna, is asymmetrically attached to the tympanic membrane. This has motivated us to solve the problem of how the middle ear influences the spatial-ambient profile and the frequency distribution of the tympanic membrane vibration. Finally, we show results from numerical simulations of the eigenfunctions and eigenfrequencies in a lizard’s internal mouth cavity bounded by the eardrums. To this end, we have constructed the complex geometry of the coupled model.

8:48 AM Y40.00005 Direct Neural Imaging using Ultra-Low Field Magnetic Resonance. KARLENE MASKALY, MICHELLE ESPY, MARK FLYNN, JOHN GOMEZ, ROBERT KRAUS, ANDREI MATLASHOV, Los Alamos National Laboratory, JOHN MOSHER, Cleveland Clinic, SHAUN NEWMAN, TUBA OWENS, MARK PETERS, J. SANDIN, LARRY SCHULTZ, ALGIS URBAITIS, PETR VOLEGOV, VAIMO ZOTEV, Los Alamos National Laboratory — An enduring challenge in neuroscience is the accurate in vivo mapping of neural activity with high spatial and temporal resolution. A method being developed by our group tries to meet this challenge by using Ultra-Low Field (ULF) MRI. Other groups have attempted direct neural imaging (DNI) using high field MRI. However, the use of ULF presents two advantages. First, the susceptibility artifact at high fields, which masks the DNI signal, is negligible at low fields. Second, the reduced Larmor frequency at ULF may overlap with the frequency spectrum of the neural magnetic field, resonantly enhancing the MRI signal. In this presentation, we will first show our custom-built ULF MRI setups that have successfully produced ULF anatomical images. I will then highlight the numerous studies we have done to investigate the feasibility of DNI with these systems, including both experimental and theoretical studies.

9:00 AM Y40.00006 Synaptic vesicle dynamics in Hippocampal Slices. KRASTAN BLAGOEV, National Science Foundation, DENIS BRAGIN, WOLFGANG MUELLER, University of New Mexico — Synaptic vesicle pool dynamics in hippocampal slices have been observed using FM-dye as an activity-dependent contrast agent with two-photon microscopy. Separate vesicle pools for spontaneous and stimulated vesicle release and vesicle dynamics, and vesicle exchange dynamics between the pools was inferred from the signal with and without stimulation. To interpret the experimental results we developed a multi-compartmental kinetic model of the FM-dye dynamics during loading and unloading of vesicles. Using this mathematical model we estimated the exchange rates between the synaptic vesicle pools and the resulting vesicle release dynamics. We will discuss important differences between the vesicle pool dynamics in ex vivo brain slices and in dissociated neuronal cultures.

9:12 AM Y40.00007 The surface properties of a lung mucus model system. MARKUS WEYGAND, BEAUTIA DEW, STEPHEN GAROFF, MATHIAS LÖSCHKE, TODD PRZBYCICHEN, ROBERT TILTON, Carnegie Mellon University — Adding surfactants to aerosol drug therapies may improve drug delivery by inducing surface tension gradient driven flows along the lung airway surfaces. Understanding the surface structure and properties of the mucus that lines the lung airways is crucial to the proper design of such formulations. In our studies, we use mucin solutions made from porcine gastric mucus as a model system. Surface tension measurements revealed a time and humidity dependence, which led us to investigate the structure of the air/solution interface using X-ray and neutron reflectivity. These studies reveal a compact adsorption layer at the air/liquid interface whose density distribution decays with a long tail extension into the bulk liquid. This structure showed only a minor dependence on the humidity above the mucus surface. To examine possible interaction between lipids present in the lung with the mucus, we deposited DPPC and DMPC onto the mucin solution surface and observed that the lipid layer remained on the solution surface for times long compared to the lifetime of mucus in the lung. The analysis of the reflectivity data impart a microscopic picture of the mucin solution surface and its alteration by lipid deposition.

9:24 AM Y40.00008 Structural Measurements from Images of Noble Gas Diffusion. ROBERT V. CADMAN, STEPHEN J. KADLECEK, KIARASH EMAMI, JOHN MACDUFFIE WOODBURN, VAHID VAHDAT, Department of Radiology, University of Pennsylvania, MASARU ISHII, Department of Otolaryngology, Johns Hopkins University, RAHIM R. RIZI, Department of Radiology, University of Pennsylvania — Magnetic resonance imaging of externally polarized noble gases such as He has been used for pulmonary imaging for more than a decade. Because gas diffusion is impeded by the alveoli, the diffusion coefficient of gas in the lung, measured on a time scale of milliseconds, is reduced compared to that of the same gas mixture in the absence of restrictions. When the alveolar walls decay, as in emphysema, diffusivity in the lung increases. In this paper, the relationship between diffusion measurements and the size of the restricting structures will be discussed. The simple case of diffusion in an impermeable cylinder, a structure similar to the upper respiratory airways in mammals, has been studied. A procedure will be presented by which airways of order 2 mm in diameter may be accurately measured; demonstration experiments with plastic tubes will also be presented. The additional developments needed before this technique becomes practical will be briefly discussed.

9:36 AM Y40.00009 Clusters of decelerations of heart rate appear to be a Hopf bifurcation, and provide early warning of illness in premature infants. ABIGAIL FLOWER, Biophysics, University of Virginia, RANDALL MOORMAN, DOUGLAS LAKE, Internal Medicine, U. Virginia, JOHN DELOS, Physics, William and Mary — The pacemaking system of the heart is complex; a healthy heart constantly integrates and responds to extracardiac signals, resulting in highly complex heart rate patterns with a great deal of variability. In the laboratory and in some pathological or age-related states, however, dynamics can show reduced complexity that is more readily described and modeled. Reduced heart rate complexity has both clinical and dynamical significance — it may provide warning of impending illness or clues about the dynamics of the heart’s pacemaking system. Here we describe uniquely simple and interesting heart rate dynamics observed in premature human infants — reversible transitions to large-amplitude periodic oscillations. We propose a mathematical interpretation based on Hopf bifurcation theory. (Supported by NIH/NIGMS, by the National Heart, Lung, and Blood Institute, and by NSF, with computing support provided by William and Mary.)

\[ \text{Supported by the U.S. NIH through grants P41-RR02305-22, R01-HL077241, and R01-HL064741.} \]
9:48AM Y40.00010 New Outlet Conditions for Three-Dimensional Computational Fluid Dynamic Simulations of Blood Flow in Arteries1, DAVID JOHNSON, Graduate Student, Dept. of Chemical Engr., ULHAS NAIK, Professor, Dept. of Chemical Engr.. In three-dimensional (3D) simulation of a component of the arterial network, we have the problem of properly specifying outlet conditions due to coupling with the rest of the arterial network. In this work we propose to use an approximate solution, based on a one-dimensional (in space) but time periodic approximation of the flow, in order to obtain these outlet conditions. These are used in fully 3D and time periodic computational fluid dynamic (CFD) simulations of a coronary arterial junction, using the commercial software Fluent. A consistent implementation requires an iterative procedure that has been developed based on a lubrication approximation. The application of these boundary conditions has been applied to both a normal/healthy coronary artery junction and a diseased case, where an occlusion has developed causing impairment of flow. Results will be shown that demonstrate significant changes to the solution.

1 NSF - IGERT Program and NASA DE Space Grant Consortium

10:00AM Y40.00011 Millimeter Wave Spectroscopy for Breast Cancer Diagnostics and Detection, KONSTANTIN KOROLEV, SHU CHEN, MOHAMMED AESAR, Tufts University, Medford, MA 02155, STEPHEN NABER, Tufts Medical Center, Boston, MA 02111 — Broad-band millimeter wave transmittance measurements of normal and tumorous (cancerous) human breast tissue samples have been acquired in–vitro by employing a free-space, quasi-optical spectrometer. Freshly excised breast tissues were prepared and preserved in 10% neutral-buffered formalin solution before testing. Significant differences in the transmittance profiles have been found between the normal and tumorous tissues. It has been found that despite the inhomogeneity and variable structure and composition of each single tissue, the tumorous specimens consistently manifest much higher absorption level of millimeter wave radiation than the normal ones. It has been shown that free space, quasi-optical spectrometer is capable of contributing valuable insights into the dielectric properties of normal and tumorous human breast tissues and aiding in further developments of millimeter wave spectroscopy and mammography for the breast cancer diagnostics and detection.

10:12AM Y40.00012 Diffusion dependence of proton NMR relaxation rates in the presence of ferritin, MICHAEL BOSS, P. CHRIS HAMMEL, The Ohio State University, Department of Physics — Ferritin is the predominant iron-storage protein in living organisms. It may serve as an indicator of neurodegenerative diseases such as Alzheimer’s. Measuring brain ferritin concentration non-invasively via MRI could enable better diagnoses and treatments of such diseases. Quantitative MRI determination of the ferritin concentration requires an understanding of the NMR relaxation mechanisms of hydrogen protons in the presence of ferritin. In aqueous solutions, ferritin enhances the transverse relaxation rate (R_2) of the protons. This is thought to occur due to a diffusive mechanism, where protons diffusing near ferritin pass through a region of elevated magnetic field, and a chemical exchange mechanism, where protons bind to the protein for a period of time, experiencing an even higher magnetic field. These two mechanisms exhibit different dependencies on the self-diffusion coefficient of the protons. By adding glycerol to aqueous solutions, we control the self-diffusion of protons. We measure the R_2 of protons in ferritin-containing binary mixtures of water and glycerol using CPMG sequences, and compare the experimental results to theoretical predictions of diffusion dependence in order to distinguish the relative importance of the mechanisms.

10:24AM Y40.00013 Application of Histogram Analysis in Radiation Therapy (HART) in Intensity Modulation Radiation Therapy (IMRT) Treatments, ANIL PYAKURYAL, Northwestern Memorial Hospital, Chicago, IL — A carcinoma is a malignant cancer that emerges from epithelial cells in structures throughout the body. It invades the critical organs, could metastasize or spread to lymph nodes. IMRT is an advanced mode of radiation therapy treatment for cancer. It delivers more conformal doses to malignant tumors sparing the critical organs by modulating the intensity of radiation beam. An automated software, HART (S. Jang et al., 2008, Med Phys 35, p. 2812) was used for efficient analysis of dose volume histograms (DVH) for multiple targets and critical organs in four IMRT treatment plans for each patient. IMRT data for ten head and neck cancer patients were exported as AAPM/RTG format files from a commercial treatment planning system at Northwestern Memorial Hospital (NMH). HART extracted DVH statistics were used to evaluate plan indices and to analyze dose tolerance of critical structures at prescription dose (PD) for each patient. Mean plan indices (n=10) were found to be in good agreement with published results for Linac based plans. The least irradiated volume at tolerance dose (TD50) was observed for brainstem and the highest volume for larynx in SIB treatment techniques. Thus HART, an open source platform, has extensive clinical implications in IMRT treatments.

10:36AM Y40.00014 Role of Physique on Probability of Injury to the Low Back, SAAMI J. SHAIBANI, Independent Modeling, Algorithms & Analytical Studies (IMMAS) — In a related study of the response of the upper and lower cervical spine[1], there was some correlation between a change in physique and the potential for injury to the neck during automotive events. A similar undertaking in this research on the lumbar spine and sacral spine revealed a much more marked effect, namely an increase in injury potential to the low back when weight is increased. Although there were some exceptions to this, the overall trend was distinct. This is perhaps to be expected when one considers that most additional weight at the same height tends to be located in the center or lower torso. However, it is first time in any comparable analysis of injury causation that there has been a more noticeable correlation between a change in physique and the potential for injury to the neck during automotive events. A similar undertaking in this research on the lumbar spine demonstrated a much more marked effect, namely an increase in injury potential to the low back when weight is increased. Although there were some exceptions to this, the overall trend was distinct. This is perhaps to be expected when one considers that most additional weight at the same height tends to be located in the center or lower torso. However, it is first time in any comparable analysis of injury causation that there has been a more noticeable correlation between a change in physique and the potential for injury to the neck during automotive events. A similar undertaking in this research on the lumbar spine demonstrated a much more marked effect, namely an increase in injury potential to the low back when weight is increased. Although there were some exceptions to this, the overall trend was distinct. This is perhaps to be expected when one considers that most additional weight at the same height tends to be located in the center or lower torso. However, it is first time in any comparable analysis of injury causation that there has been a more noticeable correlation between a change in physique and the potential for injury to the neck during automotive events. A similar undertaking in this research on the lumbar spine demonstrated a much more marked effect, namely an increase in injury potential to the low back when weight is increased. Although there were some exceptions to this, the overall trend was distinct. This is perhaps to be expected when one considers that most additional weight at the same height tends to be located in the center or lower torso. However, it is first time in any comparable analysis of injury causation that there has been a more noticeable correlation between a change in physique and the potential for injury to the neck during automotive events. A similar undertaking in this research on the lumbar spine demonstrated a much more marked effect, namely an increase in injury potential to the low back when weight is increased. Although there were some exceptions to this, the overall trend was distinct. This is perhaps to be expected when one considers that most additional weight at the same height tends to be located in the center or lower torso. However, it is first time in any comparable analysis of injury causation that there has been a more noticeable correlation between a change in physique and the potential for injury to the neck during automotive events.

11:15AM Z1.00001 Status of Experiments on the 5/2 Quantized Hall State: A Theorist’s View1, BERTRAND I. HALPERIN, Physics Department, Harvard University — A number of experiments have been proposed, which, at least in principle, should clarify the nature of the fractional quantized Hall state at filling fraction 5/2. For example, experiments might measure the spin polarization of the ground state and the charge of the elementary quasiparticles, and could test whether the quasiparticles indeed obey non-Abelian statistics, as predicted by the Moore-Read model. These experiments are difficult, however, and their interpretation may be complicated by non-uniformities in the electron density and other problems, which also pose difficulties at simpler filling fractions. We shall discuss the current experimental situation, with these issues in mind.

1 Work supported in part by a grant from the Microsoft Corporation and NSF Grant DMR 05-41988.

11:51AM Z1.00002 Fractionally charged quasiparticles at filling fraction 5/2, MOTY HEIUBLM, Weizmann Institute of Science — No abstract available.
12:27PM Z1.00003 Quasiparticle Tunneling in the Fractional Quantum Hall effect at filling fraction \( \nu = 5/2 \), IULIANA P. RADU, MIT — In a two-dimensional electron gas (2DEG), in the fractional quantum Hall regime, the quasiparticles are predicted to have fractional charge and statistics, as well as modified Coulomb interactions. The state at filling fraction \( \nu = 5/2 \) is predicted by some theories to have non-Abelian statistics, a property that might be exploited for topological quantum computation. Interferometric devices may be employed to manipulate and measure quantum Hall edge excitations. Here we use a small area edge state interferometer designed to observe quasiparticle interference effects. Oscillations in transmission consistent in detail with the Aharonov-Bohm effect are observed for integer and fractional quantum Hall states (filling factors 2, 5/3 and 7/3) with periods corresponding to their respective charges and magnetic field positions. With these charge calibrations, at filling factor 5/2 and at lowest temperatures periodic transmission through the device consistent with quasiparticle charge e/4 is observed. The principal finding of this work is that in addition to these e/4 oscillations, periodic structures corresponding to e/2 are also observed at filling factor 5/2 and at lowest temperatures. Properties of the e/4 and e/2 oscillations at 5/2 are examined with the device sensitivity sufficient to observe the relative prevalence of e/4 and e/2 oscillations, transitions between the periods, and temperature evolution of the 5/2 quasiparticle interference. Among possible etiologies, this presence of an effective e/2 period may empirically reflect an e/2 quasiparticle charge, or may reflect multiple passes of the e/4 quasiparticle around the interferometer. These results are discussed within a potential picture of e/4 quasiparticle excitations possessing non-Abelian statistics. Some critical consistencies are met between the experimental results and properties of non-Abelian e/4 quasiparticles. These studies demonstrate the capacity to perform interferometry on 5/2 excitations and reveal properties important for understanding this state and its excitations.

1:03PM Z1.00004 Measurement of filling factor 5/2 quasiparticle interference\(^1\), ROBERT WILLETT, Bell Laboratories, Alcatel-Lucent — A standing problem in low dimensional electron systems is the nature of the 5/2 fractional quantum Hall state: its elementary excitations are a focus for both elucidating the state’s properties and as candidates in methods to perform topological quantum computation. Interferometric devices may be employed to manipulate and measure quantum Hall edge excitations. Here we use a small area edge state interferometer designed to observe quasiparticle interference effects. Oscillations in transmission consistent in detail with the Aharonov-Bohm effect are observed for integer and fractional quantum Hall states (filling factors 2, 5/3 and 7/3) with periods corresponding to their respective charges and magnetic field positions. With these charge calibrations, at filling factor 5/2 and at lowest temperatures periodic transmission through the device consistent with quasiparticle charge e/4 is observed. The principal finding of this work is that in addition to these e/4 oscillations, periodic structures corresponding to e/2 are also observed at filling factor 5/2 and at lowest temperatures. Properties of the e/4 and e/2 oscillations at 5/2 are examined with the device sensitivity sufficient to observe the relative prevalence of e/4 and e/2 oscillations, transitions between the periods, and temperature evolution of the 5/2 quasiparticle interference. Among possible etiologies, this presence of an effective e/2 period may empirically reflect an e/2 quasiparticle charge, or may reflect multiple passes of the e/4 quasiparticle around the interferometer. These results are discussed within a potential picture of e/4 quasiparticle excitations possessing non-Abelian statistics. Some critical consistencies are met between the experimental results and properties of non-Abelian e/4 quasiparticles. These studies demonstrate the capacity to perform interferometry on 5/2 excitations and reveal properties important for understanding this state and its excitations.

\(^1\)collaborators L.N.Pfeiffer, K.W.West, M.Poobody

1:39PM Z1.00005 The Anti-Pfaffian and anti-Read-Rezayi States, CHETAN NAYAK, Microsoft Station Q/UCSB — No abstract available.

Friday, March 20, 2009 11:15AM - 2:15PM — Session Z2 DCMP: Detection of Non-Gaussian Noise in Mesoscopic Systems

11:15AM Z2.00001 Detection of the third moment of shot noise by a Josephson junction, JUKKA PEKOLA, Temperature Laboratory, Helsinki University of Technology — We use a hysteretic Josephson junction as an on-chip detector of shot noise of a tunnel junction. The detectable bandwidth is determined by the plasma frequency of the detector, which is about 50 GHz in the experiments that we report. The second moment of shot noise manifests itself as increased effective temperature of junction switching. The third moment results in a measurable change of the switching rate when reversing polarity of the current through the noise source. We have successfully analyzed the observed asymmetry using a phenomenological model. We compare our results to the more quantitative theories as well. Experiments on quantum point contacts and further work on tunnel junctions are in progress.

11:51AM Z2.00002 Asymmetric noise probed with a Josephson junction\(^1\), HUGUES POTHIER, Quantronics, CEA-Saclay — Using a Josephson junction, we have measured the fluctuations of the current through a tunnel junction. The current noise adds to the bias current of the Josephson junction and affects its switching out of the supercurrent branch. The experiment is carried out in a regime where switching is determined by thermal activation. The variance of the noise results in an elevated effective temperature, whereas the third moment, related to its asymmetric character, leads to a difference in the switching rates observed for opposite signs of the current through the tunnel junction. Measurements are compared quantitatively with recent theoretical predictions.

\(^1\)coauthors: Q. Le Masne, C. Urbina, Norman O. Birge, and D. Esteve

12:27PM Z2.00003 Fluctuation-induced switching and the switching path distribution, MARK DYKMAN, Michigan State University — Fluctuation-induced switching is at the root of diverse phenomena currently studied in Josephson junctions, nano-electromechanical systems, nano-magnets, and optically trapped atoms. In a fluctuation leading to switching the system must overcome an effective barrier, making switching events rare, for low fluctuation intensity. We will provide an overview of the methods of finding the switching barrier for systems away from thermal equilibrium. Generic features of the barrier, such as scaling with the system parameters, will be discussed. We will also discuss the motion of the system in switching and the ways of controlling it. Two major classes of systems will be considered: dynamical systems, where fluctuations are induced by noise, and birth-death systems. Even though the motion during switching is random, the paths followed in switching form a narrow tube in phase space of the system centered at the most probable path. The paths distribution is generally Gaussian and has specific features, which have been seen in the experiment [1]. Finding the most probable path itself can be reduced to solving a problem of Hamiltonian dynamics of an auxiliary noise-free system. The solution also gives the switching barrier. The barrier can be found exactly close to parameter values where the number of stable states of the system changes and the dynamics is controlled by a slow variable. The scaling of the barrier height depends on the type of the corresponding bifurcation. We show that, both for birth-death and for Gaussian noise driven systems, the presence of even weak non-Gaussian noise can strongly modify the switching rate. The effect is described in a simple explicit form [2,3]. Weak deviations of the noise statistics from Gaussian can be sensitively detected using balanced dynamical bridge, where this deviation makes the populations of coexisting stable states different from each other; a realization of such a bridge will be discussed. We will also discuss the sharp anisotropy of fluctuations induced by Poisson noise in overdamped systems and how it is changed with decreasing damping.

delivery by rapid injection of a large volume of DNA solution into a blood vessel, commonly called hydrodynamic gene delivery, has become a common method for gene delivery in humans. Our study employed swine as an animal model and the procedure developed includes image-guided insertion of a balloon catheter for gene therapy studies in rodents. In this presentation, I will focus on our recent work aiming at establishment of an image-guided hydrodynamic procedure. This requires solving the Kramer's problem of noise-activated escape from a metastable state beyond the Gaussian noise approximation and investigating how the measurement circuit affects threshold detection.

1:39PM Z2.00005 Theory of Josephson junction detectors of higher order noise cumulants\textsuperscript{1}. HERMANN GRABERT, Freiburg Institute for Advanced Studies — A promising strategy pursued at various laboratories to measure higher order cumulants of the electrical current of nanoscopic devices employs on-chip Josephson junction detectors. The non-Gaussian nature of the noise generated by electronic nanostructures modifies the switching rate of the Josephson junction output from the zero voltage state, and the noise cumulants can be extracted from this modification. When the decay of the metastable zero voltage state occurs by noise activation to the top of the barrier of the Josephson potential, the third noise cumulant gives rise to an asymmetry of the rate when the bias current is inverted. In the range of decay by macroscopic quantum tunneling (MQT) through the barrier potential, the forth noise cumulant leads to an enhancement of the MQT rate. The theoretical methods to describe a Josephson junction noise detector in these parameter regimes are outlined and associated experimental strategies are discussed.

\textsuperscript{1}Supported by NanoScience Programme of European Research Area (ERA)

Friday, March 20, 2009 11:15AM - 2:15PM – Session Z3 DPOLY DBP: Non-viral Based Gene Delivery Systems: Opportunities, Obstacles and Challenges 301/302

11:15AM Z3.00001 Small Bioactive Lipoplex (SBL) Nanoparticles Self-Assembled at Elevated Temperature and Pressure\textsuperscript{1}. LEAF HUANG, University of North Carolina at Chapel Hill — Conventional lipoplex (cationic liposome/DNA complex) serves well for gene transfer in cultured cells. However, their in vivo gene delivery activity is limited due to its relatively large size (~100 nm). This is due to incomplete charge neutralization as a result of the steric hindrance during the complexation between DNA and liposomes. Behr et al hypothesized that monomolecular DNA condensate can be prepared if the DNA sees the cationic lipid as monomers. Indeed, small nanoparticles (~30 nm) were prepared by using a single-chain cationic amphiphile which has a high solubility at the physiological condition. To stabilize the monomolecular condensate, Behr has included a SH group in the cationic amphiphile which could be oxidized to form a dimer. Unfortunately, the stabilized nanoparticles showed no transfection activity when delivered into cells. We hypothesized that similar small lipoplex can be prepared by using a double-chain cationic amphiphile if both DNA and the amphiphile can be soluble in the same solvent. A hydrofluorocarbon HFC-152a is an excellent solvent for the cationic lipid DOTAP at an elevated temperature (~35 °C) and pressure (~300 atm). Since the solvent can accommodate small amounts of water, DNA or siRNA could be introduced into the system to allow lipoplex formation. The resulting Small Bioactive Lipoplex (SBL) is 30-50 nm in diameter and can transfect cultured cells. Freeze-fracture electron microscopy showed that SBL are solid nanoparticles without any lipid bilayer structure. Since plasmid DNA is fragile at elevated temperature and pressure, we have concentrated our effort in siRNA which is stable under the same conditions. The new formulation shows great promise as an in vivo delivery vector when small particles are required for efficient penetration into the tissues.

\textsuperscript{1}Work supported by Eshelman Distinguished Professorship.

11:51AM Z3.00002 New Developments in Non Viral Gene Delivery. RAM MAHATO, University of Tennessee Health Science Center — No abstract available.

12:27PM Z3.00003 Image-Guided Hydrodynamic Gene Delivery, DEXI LIU, University of Pittsburgh — Gene delivery by rapid injection of a large volume of DNA solution into a blood vessel, commonly called hydrodynamic gene delivery, has become a common method for gene therapy studies in rodents. In this presentation, I will focus on our recent work aiming at establishment of an image-guided hydrodynamic procedure for gene delivery in humans. Our study employed swine as an animal model and the procedure developed includes image-guided insertion of a balloon catheter into the selected blood vessel of the targeted organ from the jugular vein and hydrodynamic injection of plasmid DNA in saline. The talk will cover the rationale of our approach, the effectiveness of procedure for gene delivery to liver and muscle, and the impact of the procedure on physiological functions and serum chemistry of the animals. The results will be discussed with respect to potential applications of the hydrodynamic gene delivery to human gene therapy.

1:03PM Z3.00004 Revisit an old problem — Complexation between DNA and PEI. CHI WU, Department of Chemistry, The Chinese University of Hong Kong — After revisiting the captioned problem by using a combination of chemical synthesis and physical methods, we studied the dynamics of the complexation between branched polyethyleneimine (iPEI) and plasmid DNA (pDNA) and characterized the structure, size and surface charge of the resultant DNA/PEI complexes (polyplexes). As expected, in order to reach a high efficiency in gene transfection into cells it is necessary to use a higher N:P ratio and make the polyplexes positively charged. Our results reveal that it is those uncomplexed iPEI chains free in the solution mixture that plays a vitally important role in enhancing the transfection efficiency, inspiring new thinking of how to correlate in vitro and in vivo studies so that we can improve the in vivo transfection efficiency. Increasing the N:P ratio normally results in a higher cytotoxicity, which is a catch-22 problem. Recently, we found that a proper modification of iPEI can greatly reduce its cytotoxicity without any suffering in the transfection efficiency. In this lecture, we will show that our properly modified iPEI is even much more effective and less cytotoxic in the gene transfection than those commercially available lipoplexes. Our recent breakthrough leads to a complete new direction in the development of non-viral vectors for molecular medicines, including gene transfection.

1:39PM Z3.00005 Recent Developments in Non-Viral Gene Delivery, ALEXANDER KABANOV, University of Nebraska Medical Center — No abstract available.

Friday, March 20, 2009 11:15AM - 2:15PM – Session Z4 DPOLY DBP: Biological Polyelectrolytes 306/307
Electrostatic Rigidity of Biological Polyelectrolytes. ANDREY DOBRYNIN, University of Connecticut — Electrostatic persistence length is one of the most controversial subjects in polymer physics. In this talk I will present an overview of the history of the problem and a new results showing that the bending rigidity of the biological polyelectrolytes ( semiflexible charged polymers) is a multiscale process. The existence of the different length scales in the bending process is manifested in change of the form of the correlation function, describing bond-bond orientational correlations, with salt concentration. At high salt concentrations when the electrostatic interactions are significantly screened these correlations may be approximated by a single exponential function indicating the existence of a dominant length scale. However, when the Debye screening length exceeds a critical value the orientational correlations between chain’s bond vectors undergo a qualitative change resulting in appearance of two different bending rigidities ( persistence lengths). One increases quadratically and the other changes logarithmically with the Debye screening length. This transition occurs when the chain’s bare persistence length becomes on the order of so-called OSF electrostatic persistence length. Simulation results and theoretical model demonstrate good qualitative agreement.

This work was done in collaboration with A. Gubarev and J.-M. Carrillo. This work was supported by the ACS Petroleum Research Fund and the Fulbright Fellowship Program.

12:27PM Z4.00003 Deafness and espin-actin self-organization in stereocilia, GERARD C.L. WONG, University of Illinois at Urbana-Champaign — Espins are F-actin-bundling proteins associated with large parallel actin bundles found in hair cell stereocilia in the ear, as well as brush border microvilli and Sertoli cell junctions. We examine actin bundle structures formed by different wild-type espin isoforms, fragments, and naturally-occurring human espin mutants linked to deafness and/or vestibular dysfunction. The espin-actin bundle structure consisted of a hexagonal arrangement of parallel actin filaments in a non-native twist state. We delineate the structural consequences caused by mutations in espin’s actin-bundling module. For espin mutation with a severely damaged actin-bundling module, which are implicated in deafness in mice and humans, oriented nematic-like actin filament structures, which strongly impinges on bundle mechanical stiffness. Finally, we examine what makes espin different, via a comparative study of bundles formed by espin and those formed by fascin, a prototypical bundling protein found in functionally different regions of the cell, such as filopodia.

In collaboration with: Kirstin Purdy-Drew; Lori Sanders; James Bartles, University of Illinois, Department of Materials Science and Engineering; Department of Physics; Department of Bioengineering.

1:03PM Z4.00004 Mesoscale Modeling of Chromatin Folding, TAMAR SCHLICK, New York University — Eukaryotic chromatin is the fundamental protein/nucleic acid unit that stores the genetic material. Understanding how chromatin fibers fold and unfold in physiological conditions is important for interpreting fundamental biological processes like DNA replication and transcription regulation. Using a mesoscale model of oligonucleosome chains and tailored sampling protocols, we elucidate the energetics of oligonucleosome folding/unfolding and the role of each histone tail, linker histones, and divalent ions in regulating chromatin structure. The resulting compact topologies reconcile features of the zigzag model with straight linker DNAs with the solenoid model with bent linker DNAs for optimal fiber organization and reveal dynamic and energetic aspects involved.

In collaboration with Gaurav Arya, S. Grigoryev, S. Correll, and C. Woodcock.

1:39PM Z4.00005 Complexation of oppositely charged polyelectrolytes in gene delivery and biology, BORIS SHKLOVSKII, University of Minnesota — Charge inversion of a DNA double helix by a positively charged flexible polymer (polyelectrolyte) is widely used to facilitate DNA contact with negative cell membranes for gene delivery. Motivated by this application in the first part of the talk I study the phase diagram a solution of long polyanions (PA) with a shorter polycations (PC) as a function the ratio of total charges of PC and PA in the solution, x, and the concentration of monovalent salt. Each PA attracts many PCs to form a complex. When x = 1, the complexes are neutral and condense in a macroscopic drop. When x is far from one, complexes are strongly charged and stable. PA are overcharged by PC at x > 1 and undercharged by PC at x < 1. As x approaches 1, PCs attached to PA disproportionate between complexes. Some complexes become neutral and condensed in a macroscopic drop while others become even stronger charged and stay free. The second part of the talk deals with biological example of PA - PC complexes namely self-assembly of vegetable viruses from long ss-RNA molecule paying role of scaffold and identical capsid proteins with long positive tails. I show that optimization Coulomb energy of the virus leads to the charge of virus twice larger than the charge of the capsid, in agreement with the experimental data. Then I discuss kinetics of the Coulomb complexation driven virus self-assembly. Capsid proteins stick to un assembled chain of ss RNA (which we call “antenna”) and slide on it towards the assembly site. I show that at excess of capsid proteins such one-dimensional diffusion accelerates self-assembly more than ten times. On the other hand at excess of ss-RNA, antenna slows self-assembly down. Several experiments are proposed to verify the role of ss-RNA antenna in self-assembly.
suggesting intriguing possibilities for genetic analysis.

The basic principle behind this is that when DNA is electrophoretically driven through a nanopore, it blocks a measurable fraction of the current. Our work also focuses on solid-state nanopores, single-nanometer-scale devices that can not only manipulate single molecules, but also can manipulate long DNA molecules by a variety of nanoscale phenomena, including electrokinetics, hydrodynamics, Coulomb interactions, and the statistical mechanics of polymers.

As we shrink fluidic devices down to the nanoscale to probe samples as minute as a single molecule, what physical phenomena grew increasingly important. As we shrink fluidic devices down to the nanoscale to probe samples as minute as a single molecule, what physical phenomena grew increasingly important. As we shrink fluidic devices down to the nanoscale to probe samples as minute as a single molecule, what physical phenomena grew increasingly important. As we shrink fluidic devices down to the nanoscale to probe samples as minute as a single molecule, what physical phenomena grew increasingly important.

One of the most dramatic manifestations of the quantum nature of light in the past half-century has been the Casimir force: a force between neutral objects at close separations caused by quantum vacuum fluctuations in the electromagnetic fields. In classical photonics, wavelength-scale structures can be designed to dramatically alter the behavior of light, so it is natural to consider whether analogous geometry-based effects occur for Casimir forces. However, this problem turns out to be surprisingly difficult for all but the simplest planar geometries. (The deceptively simple case of an infinite plate and infinite cylinder, for perfect metals, was first solved in 2006.) Many formulations of the Casimir force, indeed, correspond to impossibly hard numerical problems. We will discuss how the availability of large-scale computing resources in NSF's TeraGrid, combined with reformulations of the Casimir-force problem oriented towards numerical computation, are enabling the exploration of Casimir forces in new regimes of geometry and materials.

We acknowledge financial support from Boston University.

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MICHAEL ROUKES, California Institute of Technology — Mass spectrometry (MS) has become a preeminent methodology of proteomics since it provides rapid and quantitative identification of protein species with relatively low sample consumption. Yet with the trend toward biological analysis at increasingly smaller scales, ultimately down to the volume of an individual cell, MS with few-to-single molecule resolution will be required. We report the first realization of MS based on single-molecule mass spectrometry providing proof-of-principle for this new technique. Nanoparticles and protein species are introduced by electrospray injection from the fluid phase into ambient conditions into vacuum and subsequently delivered to the NEMS detector by hexapole ion optics. Mass measurements are then recorded in real-time as analytes adsorb, one-by-one, onto a phase-locked, ultrahigh frequency (UHF) NEMS resonator. These first NEMS-MS spectra, obtained with modest resolution from only several hundred mass adsorption events, presage the future capabilities of this methodology. We outline the substantial improvements feasible in near term, through recent advances and technological avenues that are unique to NEMS-MS.

1:03PM Z7.00004 Using Photoactivation Light Microscopy (PALM) to construct comprehensive, nanometer precision atlases of signaling complexes

JAN LIPHARDT, University of California, Berkeley — The E. coli chemotaxis network is a model system for biological signal processing. In E. coli, transmembrane receptors responsible for signal transduction assemble into large clusters containing several thousand proteins. These sensory clusters have been observed at cell poles and future division sites. Despite extensive study, it remains unclear how chemotaxis clusters form, what controls cluster size and density, and how the cellular location of clusters is robustly maintained in growing and dividing cells. Here we use photoactivated localization microscopy (PALM) to map the cellular locations of three proteins central to bacterial chemotaxis (the Tar receptor, CheY, and CheW) with a precision of 15 nanometers. We find that cluster sizes are approximately exponentially distributed, with no characteristic cluster size. One third of Tar receptors are part of smaller lateral clusters and not the large polar clusters. Analysis of the relative cellular locations of 3.1 million individual proteins (from 326 cells) suggests that clusters form via stochastic self-assembly. The super-resolution PALM maps of E. coli receptors support the notion that stochastic self-assembly can create and maintain approximately periodic structures in biological membranes, without direct cytoskeletal involvement or active transport.

1:39PM Z7.00005 Single-molecule dynamics in nanofabricated traps

ADAM COHEN, Harvard University — The Anti-Brownian Electokinetic trap (ABEL trap) provides a means to immobilize a single fluorescent molecule in solution, without surface attachment chemistry. The ABEL trap works by tracking the Brownian motion of a single molecule, and applying feedback electric fields to induce an electokinetic motion that approximately cancels the Brownian motion. We present a new design for the ABEL trap that allows smaller molecules to be trapped and more information to be extracted from the dynamics of a single molecule than was previously possible. In particular, we present strategies for extracting dynamically fluctuating mobilities and diffusion coefficients, as a means to probe dynamic changes in molecular charge and shape. If one trapped molecule is good, many trapped molecules are better. An array of single molecules in solution, each immobilized without surface attachment chemistry, provides an ideal test-bed for single-molecule analyses of intramolecular dynamics and intermolecular interactions. We present a technology for creating such an array, using a fused silica plate with nanofabricated dimples that have removable cover for sealing single molecules within the dimples. With this device one can watch the shape fluctuations of single molecules of DNA or study cooperative interactions in weakly associating protein complexes.

Friday, March 20, 2009 11:15AM - 2:15PM

Session Z8 DBP: Statistical Physics in Biology 414/415

11:15AM Z8.00001 Allometric Scaling in Biology

JAYANTH BANAVAR, Penn State — The unity of life is expressed not only in the universal basis of inheritance and energetics at the molecular level, but also in the pervasive scaling of traits with body size at the whole-organism level. More than 75 years ago, Kleiber and Brody and Proctor independently showed that the metabolic rates, B, of mammals and birds scale as the three-quarter power of their mass, M. Subsequent studies showed that most biological rates and times scale as $M^{-1/4}$ and $M^{1/4}$, respectively, and that these so-called quarter-power scaling relations hold for a variety of organisms, from unicellular prokaryotes and eukaryotes to trees and mammals. The wide applicability of Kleiber’s law, across the 22 orders of magnitude of body mass from minute bacteria to giant whales and sequoias, raises the hope that there is a relationship between metabolic rate, B, and body mass, M. We show how the pervasive quarter-power biological scaling relations arise naturally from optimal directed resource supply systems. This framework robustly predicts that: 1) whole organism power and resource supply rate, B, scale as $M^{5/4}$; 2) most other rates, such as heart rate and maximal population growth rate scale as $M^{-1/4}$; 3) most biological times, such as blood circulation time and lifespan, scale as $M^{1/4}$; and 4) the average velocity of flow through the network, $\bar{v}$, such as the speed of blood and oxygen delivery, scales as $M^{1/12}$. Our framework is valid even when there is no underlying network. Our theory is applicable to unicellular organisms as well as to large animals and plants. This work was carried out in collaboration with Amos Maritan along with Jim Brown, John Damuth, Melanie Moses, Andrea Rinaldo, and Geoff West.

11:51AM Z8.00002 From gene expressions to genetic networks

MAREK CIEPLAK, Institute of Physics, Polish Academy of Sciences — A method based on the principle of entropy maximization is used to identify the gene interaction network with the highest probability of giving rise to experimentally observed transcript profiles [1]. In its simplest form, the method yields the pairwise gene interaction network, but it can also be extended to deduce higher order correlations. Analysis of microarray data from genes in Saccharomyces cerevisiae chemostat cultures exhibiting energy metabolic oscillations identifies a gene interaction network that reflects the intracellular communication pathways. These pathways adjust cellular metabolic activity and cell division to the limiting nutrient conditions that trigger metabolic oscillations. The success of the present approach in extracting meaningful genetic connections suggests that the maximum entropy principle is a useful concept for understanding living systems, as it is for other complex, nonequilibrium systems. The time-dependent behavior of the genetic network is found to involve only a few fundamental modes [2,3].

REFERENCES:


12:27PM Z8.00003 Non-equilibrium thermodynamic effects during cell division, JORGE JOSE, SUNY at Buffalo — A mitotic spindle is a regular structure within a cell consisting of oriented microtubule fibers. It plays a fundamental role in chromosome separation during cell division. Forming a spindle pattern is a major structural step towards mitosis. We have developed biophysical non-equilibrium thermodynamic models to describe in vitro chromosome driven spindle formation experiments in Xenopus extracts. Our first 2D model calculations [1] successfully described the order of events seen in some of the Xenopus extracts experiments, where the chromosomes are replaced by chromatin-covered micrometer magnetic beads. I will describe more realistic 3D improvements in our modeling analysis, which include microtubule contact forces and excluded volume [2, 3]. There are, however, a number of challenges that must be addressed for spindle modeling to continue to be a useful tool for understanding this fundamental biological process, in particular the biophysical simulation times. In this talk I will describe some important problems needing better biological data and hypothesis. I will also discuss our most recent numerical algorithmic improvements that are expected to greatly increase the simulations speed and thus allowing a more realistic representation of the experimental situation in Xenopus extracts. [1] S. C. Schaffner and J. V. Jose, PNAS, 103, 11166 (2006), [2] ibid in “Methods in Cell Biology” (Elsevier-Academic Press)(2008)and [3]ibid(to be published).

1:03PM Z8.00004 New Proposed Mechanism for Actin-Polymerization-Driven Motility1, ANDREA LIU, University of Pennsylvania — When a cells crawls, its shape re-organizes via polymerization and depolymerization of a network of actin filaments. The growing ends of the filaments are localized near the leading edge of the crawling cell, and their polymerization, regulated by a host of proteins, pushes the cell membrane forwards in a biological model known as the dendritic nucleation model. We have performed Brownian dynamics simulations to see how the dendritic nucleation model leads to motion. Our results are not consistent with previous models of motility, and suggest a new picture for the physical mechanism underlying this form of motility.

1:39PM Z8.00005 to be determined by you, DANIEL ROKHSAR, TBD — No abstract available.

Friday, March 20, 2009 11:15AM - 2:15PM –
Session Z9 GSNP: Nonlinear Dynamics and Chaotic Systems 303

11:15AM Z9.00001 Rotating Space Elevator: Classical and Statistical Mechanics of cosmic scale spinning strings1, STEVEN KNUDSEN, LEONARDO GOLUBOVIC, West Virginia University — We introduce a novel and unique nonlinear dynamical system, the Rotating Space Elevator (RSE). The RSE is a multiply rotating system of cables (strings) reaching beyond the Earth geo-synchronous satellite orbit. Strikingly, objects sliding along the RSE cable do not require internal engines or propulsion to be transported far away from the Earth’s surface. The RSE actio employs, in a very fundamental way, basic natural phenomena – gravitation and inertial forces. The RSE exhibits interesting nonlinear dynamics and statistical physics phenomena. Its kinetic phase diagram involves both chaotic and quasi-periodic states of motion separated by a morphological phase transition that occurs with changing the RSE angular frequency.

1We thank NASA and WVHTC for the grant WVHTC-W-NASA-IR-06-1330: Innovative Research Technologies for Next Generation Space Exploration.

11:27AM Z9.00002 Numerical investigation on the chaos assisted tunneling for a coupled microwave cavity1, HOSHIK LEE, Temple University, LOUIS PECORA, DONG HO WU, Naval Research Laboratory — It is known that chaos-assisted dynamical tunneling may occur in nonintegrable (chaotic) systems. Recently we investigate wave chaotic systems to see if the system may promote the chaos-assisted spatial tunneling in addition to the dynamic tunneling. Our previous experiments suggest some enhancement of the spatial tunneling rate in a coupled, wave-chaotic 2D microwave double cavity, indicating that the presence of chaotic modes changes not only the dynamical tunneling rate but also the spatial tunneling rate. To understand the underlying physics we carry out numerical simulations on nonintegrable 2D cavities as well as on integrable 2D cavities. We will present details about the experiments and numerical simulation results.

11:39AM Z9.00003 Scaling properties of delay times in one-dimensional random media1, JOSHUA BODYFELT, Department of Physics, Wesleyan University, Middletown, Connecticut, ANTONIO MENDEZ-BERMUDEZ, Instituto de Fisica, Universidad Autonoma de Puebla, Puebla, Mexico, ANDREY CHABANOV, Department of Physics and Astronomy, The University of Texas at San Antonio, Texas, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown, Connecticut — The scaling properties of the inverse moments of Wigner delay times are investigated in finite one-dimensional (1D) random media with one channel attached to the boundary of the sample. We find that they follow a simple scaling law which is independent of the microscopic details of the random potential. Our theoretical considerations are confirmed numerically for systems as diverse as 1D disordered wires and optical lattices to microwave waveguides with correlated scatterers.

1This research was supported by a grant from the United States-Israel Binational Science Foundation (BSF), Jerusalem, Israel.

11:51AM Z9.00004 Lyapunov exponent calculation via reconstruction of the invariant density function from iterative Chebyshev maximum entropy approach1, NAGENDRA DHAKAL, HIRO SHIMOYAMA, PARTHAPRATIM BISWAS, The University of Southern Mississippi — We apply a maximum entropy approach (MaxEnt) to compute invariant density functions to obtain the Lyapunov exponents. The method gives the solution by iteratively calculating the Lagrange multipliers within the maximum entropy method from moment constraints. We illustrate our method by reproducing known invariant densities for several cases of discrete maps (in both chaotic and non-chaotic regimes). The global convergence of invariant density function is studied with particular emphasis on Lyapunov exponent of the map by varying number of moments. We demonstrate that Lyapunov exponent of a chaotic map can be computed with a high degree of precision from this approach.

1University of Southern Mississippi, Grant No. DE00945
12:03PM Z9.00005 Time-Shifted Synchronization of Chaotic Oscillator Chains without Explicit Coupling Delays

Jonathan Blakey, Mark Stahl, Ned Corron, US Army RDECOM — It has recently been reported that time-shifted synchronization (i.e., lag or anticipation) of chaotic oscillators can result from forms of coupling that do not contain explicit delay terms. Identical time-shifted synchronization is not a solution in these systems so the dynamics are a form of generalized synchronization where trajectories are similar but not exactly identical. Here we examine chains of unidirectionally coupled oscillators in which time-shifted synchronization occurs without delays in the coupling. We observe the distortion of the waveforms of the response oscillators located far from the drive oscillator. Under weak coupling, we see much less distortion occurs over chains with significant total time shift than predicted by a recently introduced theoretical estimate. Under stronger coupling, we find better agreement with the theoretical prediction and, despite sometimes severe attenuation, propagation structure is maintained even over long chain lengths. We report results from numerical models as well as from an experimental system of electronic circuits. Such oscillator chains may prove useful in applications requiring a variable delay such as chaotic radar or beam forming.

12:15PM Z9.00006 Combining Wave Chaos and the Loschmidt Echo to Extend the Concept of Fidelity to Classical Waves

Dmitry V. Dynlov, Jason W. Fleischer, Princeton University, Princeton, NJ 08544, USA — We experimentally and theoretically consider a double-bump-on-tail instability of a classical laser system by applying the wave mechanical concept of fidelity loss to classical waves. The sensor makes explicit use of time-reversal invariance and spatial reciprocity in a wave chaotic system to sensitively and remotely measure the presence of small perturbations to the system. The loss of fidelity is measured through a classical wave-analog of the Loschmidt echo by employing a single-channel time-reversal mirror to rebroadcast a probe signal into the perturbed system. We also introduce the use of exponential amplification of the probe signal to partially overcome the effects of propagation losses. It is demonstrated that exponential amplification can be used to vary the spatial range of sensitivity to perturbations, thereby actively modifying the range of operation of the sensor. Experimental results are presented for both electromagnetic and acoustic versions of the Loschmidt echo based sensor.

12:27PM Z9.00007 Synchronization and Competition in a Double-Bump-on-Tail Instability

DMITRY V. DYLOV, JASON W. FLEISCHER, Princeton University, Princeton, NJ 08544, USA — We experimentally and theoretically consider a double-bump-on-tail instability by mapping the general wave-kinetic problem to a multiple beam propagation problem using statistical light. More specifically, we consider the nonlinear interaction of three spatially-incoherent beams in a self-focusing photoconstructive crystal. For weak nonlinearity, we observe instability competition and sequential flattening of the bumps in momentum space, with no observable variations in position-space intensity. This joint dynamics resembles the phase synchronization of a “classical” laser system (relaxation to a lower-energy state) with the corresponding intensity modulations appearing from the optical equivalent of inverse Landau damping. For strong nonlinearity, intensity modulations appear and the triple-hump spectrum merges into a single-peaked profile with an algebraic $k^{-2}$ inertial range. This spectrum, with its associated modulations, is a definitive observation of soliton, or Langmuir, turbulence.

12:39PM Z9.00008 Stratospheric Ozone and Dynamical Systems

FRANCISCO J. URIBE, ROSA MARIA VELASCO, ERNESTO PEREZ-CHAVELA, Universidad Autonoma Metropolitana — We consider the Chapman mechanism for stratospheric ozone dynamics. The resulting nonlinear differential equations are studied from the point of view of the theory of dynamical systems. In particular we calculate and analyze the nature of the critical points and show that the region in which the concentrations are non-negative is a positively invariant set, meaning that initial conditions with non-negative concentrations always give non-negative concentrations. Poincaré compactification is used to elucidate the global flow. Comments about the inclusion of nitrogen oxides are also given.

1:03PM Z9.00010 Scattering a pulse from a chaotic cavity: Transitioning from algebraic to exponential decay

James Hart, Thomas Antonsen, Edward Ott, University of Maryland — The ensemble averaged power scattered in and out of lossless chaotic cavities (such as microwave resonators, acoustic cavities and quantum dots) decays as a power law in time for large times. In the case of a pulse with a finite duration, the power scattered from a single realization of a cavity closely tracks the power law ensemble decay initially, but eventually transitions to an exponential decay. In this presentation, we explore the nature of this transition in the case of coupling to a single port. We find that for a given pulse shape, the properties of the transition are universal if time is properly normalized. We define the crossover time to be the time at which the deviations from the mean of the reflected power in individual realizations become comparable to the mean reflected power. We demonstrate numerically that, for randomly chosen cavity realizations and given pulse shapes, the probability distribution function of reflected power depends only on time, normalized to this crossover time. Paper: http://arxiv.org/abs/0810.1664

1:15PM Z9.00011 Stability of large complex systems

Harold Hastings, Hofstra University — We use a random matrix model to study the stability of large, complex systems. Our approach was motivated by a long-standing dilemma concerning stability of large systems. MacArthur (1955) and Hutchinson (1959) argued that more “complex” natural systems tended to be more stable than less complex systems based upon energy flow. May (1972) argued the opposite, using random matrix models. In prior work we showed that in some sense both are right: under reasonable scaling assumptions on interaction strength, Lyapunov stability increases but structural stability decreases as complexity is increased (c.f. Harrison, 1979; Hastings, 1984). We now apply these methods to a variety of complex systems.

1:27PM Z9.00012 Synchronization Delays and Fidelity of State Change in Chaotic Systems

Dmitry V. Dynlov, Jason W. Fleischer, Princeton University, Princeton, NJ 08544, USA — Time-reversal mirrors have been successfully used to demonstrate time-reversal invariance in a number of different situations. By employing a two-channel time-reversal mirror scheme, we have experimentally demonstrated that the Loschmidt echo is a universal phenomenon for chaotic systems. In this presentation, we investigate the effect of time delays on the Loschmidt echo. We show that, for randomly chosen cavity realizations and given pulse shapes, the probability distribution function of reflected power depends only on time, normalized to this crossover time. Paper: http://arxiv.org/abs/0810.1664

1:39PM Z9.00013 Stability of large complex systems

Harold Hastings, Hofstra University — We use a random matrix model to study the stability of large, complex systems. Our approach was motivated by a long-standing dilemma concerning stability of large systems. MacArthur (1955) and Hutchinson (1959) argued that more “complex” natural systems tended to be more stable than less complex systems based upon energy flow. May (1972) argued the opposite, using random matrix models. In prior work we showed that in some sense both are right: under reasonable scaling assumptions on interaction strength, Lyapunov stability increases but structural stability decreases as complexity is increased (c.f. Harrison, 1979; Hastings, 1984). We now apply these methods to a variety of complex systems.

1Partially supported by DOE grant DE-FG02-08ER64623 for the Hofstra University Center for Condensed Matter Research.
1.27PM Z9.00012 The Initiation of Optical Breakdown in Simple Liquids, KEVIN CISSNER, Air Force Research Laboratories — The probability of breakdown in 40 simple HPLC hydrocarbons and water from a Q-switched laser at 1064 (6ns) and 532 nm (5 ns) was measured using a variety of lenses and cell path length. In each instance a plot of the cumulative distribution function vs. the input laser fluence fits an error-function well, except at low probabilities. Care was taken to measure the light distribution in situ across the entire focal plane. The transmission within the HOMO-LUMO gap was also measured using the long-path-length cells. Trends in the breakdown data with the optical/electronic properties of the target liquids are confounded by spherical aberration. However, the data suggest a connection to the chemical group of the liquid and especially to the C-X bond. In all cases the threshold at 1064 nm is actually less than that at 532 nm. No evidence was found for a mechanism involving dissolved air. A comparison is made to the behavior for static breakdown in gases.

1.39PM Z9.00013 Analysis of Laser Breakdown Data, ROGER BECKER, Air Force Research Labs — Experiments on laser breakdown for ns pulses of 532 nm or 1064 nm light in water and dozens of simple hydrocarbon liquids are analyzed and compared to widely-used models and other laser breakdown experiments reported in the literature. Particular attention is given to the curve for the probability of breakdown as a function of the laser fluence at the beam focus. Criticism is made of the naive forms of both “avalanche” breakdown and multi-photon breakdown. It appears that the process is complex and is intimately tied to the chemical group of the material. Difficulties with developing an accurate model of laser breakdown in liquids are outlined.

1.51PM Z9.00014 Fidelity Gap in Dynamical Systems with Critical Chaos, CARL T. WEST, Department of Physics, Wesleyan University, Middletown, Connecticut 06459, USA and MPI for Dynamics and Self-Organization, 37073 Goettingen, Germany — We analyze the fidelity decay for a class of dynamical systems showing critical chaos, using a Kicked Rotor with singular kicking potential as a prototype model. We found that the classical fidelity shows a gap $F_0$ (initial drop of fidelity) which scales as $F_0(\alpha, \epsilon, \eta) = \chi(\epsilon \equiv \frac{2\pi}{\alpha\eta})$ where $\alpha$ is the order of singularity of the non-analytical potential, $\eta$ is the characteristic spread of the initial phase space density and $\epsilon$ is the perturbation strength. Instead, the corresponding quantum fidelity gap is insensitive to $\alpha$ due to strong diffraction effects that dominate the quantum dynamics.

3This research is supported by the National US-Israel Science Foundation (BSF) and by the DFG FOR-760.

2.03PM Z9.00015 Irreversibility, Poincare Recurrence and Stochasticity in Statistical Mechanics, PURU GUJRATI, The University of Akron — We will show that deterministic dynamics always leads to the conservation of entropy and Poincare recurrence. Thus, recurrence is incompatible with entropy change. The law of increase of entropy can only occur for systems with stochastic dynamics, and the irreversibility emerges out of their indeterminate evolution as we will discuss. This stochasticity requires some weak but uncontrollable interaction of the system outside or the walls of the container. Boltzmann incurs this stochasticity in his deterministic approach by invoking the assumption of molecular chaos. The molecular chaos cannot emerge out of deterministic dynamics, as shown elsewhere in this meeting.


3Pradeep Fernando and P.D. Gujrati (poster)


11:15AM Z10.00001 Dielectric properties of cluster-deposited TiO$_2$ nanocomposites, B. BALAMURUGAN, University of Nebraska, KRISTIN KRAEMER, University of Nebraska, X. WEI, University of Nebraska, STEPHEN DUCHARME, University of Nebraska, D.J. SELLMYER, University of Nebraska — TiO$_2$-polymer nanocomposites are expected to have a high dielectric permittivity of TiO$_2$ and large breakdown strength of the polymer, resulting in high energy density suitable for energy storage devices. Since chemically prepared nanocomposites tend to have poor film quality and inhomogeneities due to agglomeration, cluster deposition technique was used to prepare monodispersed TiO$_2$-paraffin nanocomposite films. TiO$_2$ clusters were coated in-flight with paraffin wax having comparatively better dielectric strength (7.9 – 11.8 MV/m) using a thermal evaporation source in prior to deposition. Bare TiO$_2$ clusters with average particle size ranging from 8 to 12 nm having a maximum dielectric permittivity of 54 were obtained. The structural and dielectric properties of these nanocomposites with varying volume fractions will be discussed. This research is supported by ONR and NCMN.

11:27AM Z10.00002 Lattice Dielectric and Thermodynamic Properties of Yttria Stabilized Zirconia (YSZ) Solids, KAH CHUN LAU, Department of Chemistry, George Washington University, Washington D.C. 20052, BRETT I. DUNLAP, Code 6189, Naval Research Laboratory, Washington D.C. 20375 — A study of lattice dielectric and thermodynamic properties of Yttria Stabilized Zirconia (YSZ) solids as a function of yttria concentration is reported. Within the local density approximation (LDA) and the harmonic approximation, we find excellent agreement between calculated and experimental specific heat and dielectric constants. From the variation of the specific heat of YSZ with yttria composition, we propose a simple additive rule that estimates the dependence of the specific heat of YSZ on yttria concentration. Whereas for the dielectric constants of YSZ, the values are bounded by the dielectric constants of the cubic and amorphous zirconia.

1This work is supported by the Office of Naval Research, both directly and through the Naval Research Laboratory.

11:39AM Z10.00003 Space-Charge-Limited Conduction Under Trap Density Gradient Exhibiting Bulk-Limited Diode, YUKIO WATANABE, Kyushu Univ. — Space-charge-limited (SCL) conduction in the presence of a trap density gradient is studied theoretically, which is compared with experiments in detail. Under this condition, the current ($J$) – voltage ($V$) characteristics at low voltage are ohmic and symmetric with respect to the bias polarity. At high voltage, $JV$ characteristics follow the $J \propto V^m \left(1 \leq m \leq 2\right)$ law at both polarities and are asymmetric with respect to the bias polarity. These characteristics have not been reported in the previous studies and agree well with experiments. These agreements verify that a bulk-limited conduction can exhibit rectifying, i.e., diode-like $JV$ characteristics without relying on Schottky barriers and diffusion currents. The theory is presented in easily tractable algebraic recurrence formulae and reproduces experimental $JV$ characteristics excellently using three free parameters, only one more than that used in standard SCL theory.

1We acknowledge Grants-in-aid for Scientific Research from JSPS No. 19340084
11:51AM Z10.00004 Optical second-harmonic generation measurements of porous low-k dielectric materials

JOANNA ATKIN, Columbia University, THOMAS SHAW, IBM Yorktown, ROBERT LAIBOWITZ, TONY HEINZ, Columbia University — Low-k dielectric materials based on porous carbon-doped oxides, with relative dielectric constants as low as 2.1, are widely used as thin insulating films in the microelectronics industry. Knowledge of these materials’ basic electronic properties, such as energy gaps, barrier heights, and trap states, is essential for modeling their electrical leakage and stability characteristics. We use femtosecond laser pulses to probe the dynamics of charge-carrier transfer processes across Si/LKD interfacial barriers by optical second harmonic generation (SHG). Larger electric fields from multiphoton injection can be developed in Si/LKD systems compared to Si/SiO2, indicating a significantly higher density of traps in the LKD. This is consistent with previously reported measurements of trap density by photoinjection techniques alike. We will also discuss results on the dynamics of discharging and on the dependence of charging phenomena on layer thickness. * J. M. Atkin, D. Song, T. M. Shaw, E. Cartier, R. B. Laibowitz, and T. F. Heinz, J. Appl. Phys. 103, 094104 (2008).

1Supported by the Semiconductor Research Corporation

12:03PM Z10.00005 Energy-band parameters of atomic-layer-deposited Al2O3 and HfO2 on InxGa1-xAs

M.L. HUANG, Y.C. CHANG, Y.H. CHANG, T.D. LIN, M. HONG, J. KWO, National Tsing Hua University, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING TEAM, DEPARTMENT OF PHYSICS TEAM — X-ray photoelectron spectroscopy (XPS) combined with reflection electron energy loss spectroscopy (REELS) were used to determine the energy-band parameters, valence-band offsets ΔEv, conduction-band offsets ΔEc, and energy-band gap Es, of the atomic layer deposited (ALD) high k dielectrics of Al2O3 and HfO2 on InxGa1-xAs (x=0, 0.15, 0.25, and 0.53). Using REELS, Eg values of the ALD-Al2O3 and -HfO2 were estimated to be 6.77 and 5.56 ±0.05 eV, respectively. The ΔEv’s and ΔEc’s are larger than 1.5 and 2.5 eV, respectively, for all the ALD-oxide/InGa1-xAs samples. The ΔEc values obtained from the HR-XPS and REELS analyses are in good agreement with those estimated from the electrical measurement according to Fowler-Nordheim tunneling. The results are valuable to the understanding and modeling of the III-V high k MOS devices.

12:15PM Z10.00006 Resonant photo-ionization of charged oxygen vacancy defects in Si/SiO2/HfO2 film stacks observed by second-harmonic generation.

J. PRICE, M. C. DOWNER, University of Texas, Austin — The semiconductor industry recently achieved a historic milestone with the introduction of high-k gate dielectrics. However, much effort continues to focus on characterizing defects in these materials that promote charge trapping. Using internal multi-photon photoemission (IMPE) and time-dependent electrostatic field-induced second harmonic (TD-EFISH) generation, we probe the charge trapping kinetics in Si/SiO2/HfO2 gate stacks. During IMPE charging, the TD-EFISH response of the HfO2 film uniquely increases and then decreases when irradiated at the characteristic three-photon energy of 4.71 eV. The decrease in TD-EFISH is explained by resonant three-photon excitation of HfO2-induced negatively charged oxygen vacancy defects in the SiO2 interfacial layer, and subsequent removal of its negative charge by tunneling to the Si substrate. This interpretation is supported by spectroscopic ellipsometry and electron spin resonance measurements, and ab initio calculations, which identify the 4.71 eV transition with this defect. Photo-ionization of this defect also explains hysteresis in the TD-EFISH response when charges trapped at the surface are quenched between successive IMPE charging cycles. The results demonstrate that second harmonic generation can potentially be used as an in situ, real time monitor of charge trapping kinetics prior to device fabrication.

12:27PM Z10.00007 Combined theoretical and experimental study of thin hafnia films

XUHUI LUO, ALEXANDER A. DEMKOV, The University of Texas, DINA TRIYSO, PETER FEJES, RICH GREGORY, STEFAN ZOLLNER, Freescale Semiconductor, Inc. — Hafnia-based dielectric films have replaced silica as a gate dielectric in field effect transistors. We present a joint experimental and theoretical study of ultra thin hafnia films grown on Si (001) by atomic layer deposition. Using density functional theory we investigate the surface energy of monoclinic and tetragonal hafnia films in search for thermodynamic means of controlling the film microstructure. Our calculations of the surface phase diagram reveal that in the absence of hydrogen (111), and (111) are the lowest energy surface terminations of monoclinic hafnia under a wide range of chemical environment. On the other hand, the structural analysis, indicates films with thickness of 4 nm or less to be polycrystalline, predominantly monoclinic with the texture axis being normal to the (211), (112). Our calculations suggest that under oxygen rich conditions the (112) termination can be stabilized. Furthermore, we discuss the effects of the hydroxylation on the thermodynamics of the hafnia film grown by ALD and provide a new perspective into the dynamics of the film growth.

1Supported in part by the NSF under grant DMR-0606464

12:39PM Z10.00008 Resonant Localized Nanoplasma in Oblique Far Infrared Reflectivity of Transition Metal Granular Films

N.E. MASSA, LANAINA EFO-CEQINOR, ULP, CC 962, 1900 La Plata, Argentina, J.C. DENARDIN, Dpto de Física, USACh, Santiago, Chile, L.M. SOCOLOVSKY, ITCI ,UBA, Buenos Aires, Argentina, M. KNOBEL, Inst. de Física, UNICAMP, Campinas, Brazil, X.X. ZHANG, INST- HKUST, Hong Kong, China — We report on near normal and angle dependent specular infrared reflectivity of transition metal and SiO2 cosputtered nanogranular ~550 nm thick films in the insulating regime. Their reflectivity is characterized by well defined vibrational bands, an overdamped Drude contribution, due to carriers denoting the existence of conducting critical paths not yet truncated, and a distinctive band at ~1450 cm⁻¹ originating in electron promotion, localization, and polaron formation. (TM) P-polarized oblique reflectivity, as from globally isolating Co3(38)SiO2(30.62)Fe3(34)SiO2(30.66) or Ni(28)SiO2(70.2), reveals a remarkable resonance at the ~1450 cm⁻¹ band threshold. Its maximum intensity is reached at the radiation tangential component null condition allowing for a collective electronic excitation induced as localized plasma. It is attributed to carriers that are not able to overcome the metal-dielectric rough interface. As the angle of incidence increases the longitudinal highest frequency vibrational band merges with the P-polarized resonance inducing broadening and softening reminiscent to lattice modes undergoing strong electron-photon interactions.

12:51PM Z10.00009 Phase Equilibrium of Size-Dispersed Colloid Systems with soft pair interactions: A Monte Carlo Study

JOANNIS BITSANIS, FORTH-IESL, Heraklion, Greece, IOANNIS ECONOMOY, MARIANNA YIANNOUKAKOU, NRCPs “Demokritos”, Ag. Paraskevi, Greece — We have studied the solid-fluid coexistence for systems of polydisperse soft spheres that interact via power-law potentials. We employed isobaric semi-grand ensemble simulations. Gibbs-Duhem integration traced the coexistence pressure as a function of the breadth of particle variance of the imposed activity distribution. Fluid-solid coexistence densities were determined to be monotonically increasing functions of the breadth of particle size dispersion, and ab initio calculations, which identify the 4.71 eV transition with this defect. Photo-ionization of this defect also explains hysteresis in the TD-EFISH response when charges trapped at the surface are quenched between successive IMPE charging cycles. The results demonstrate that second harmonic generation can potentially be used as an in situ, real time monitor of charge trapping kinetics prior to device fabrication.
**1:03PM Z10.00010 First-principles simulations of extended phosphorus oxynitride structures in LiPON glasses**¹, YAOJUN DU, N. A. W. HOLZWARTH, Wake Forest University — The thin film electrolyte LiPON, having the composition of Li$_{1.2}$PO$_{1.5}$F$_x$N$_{1-x}$ with $x = 3z - 2y$, was developed at Oak Ridge National Lab in the 1990’s for use in solid state batteries and related applications. In an effort to understand and to optimize properties of this electrolyte material, we expanded previous studies of isolated defects in crystalline Li$_{1.2}$PO$_{1.5}$F$_x$N$_{1-x}$ to focus on more complicated phosphate structures based on combinations of tetrahedral P–O bonds and bridging P=O–P bonds. For example, crystalline Li$_{1.2}$PO$_{1.5}$F$_x$N$_{1-x}$ and P$_2$O$_5$ are composed of phosphate structures with linear and branched chains, respectively. Both these and related structures derived from substituting O with N and adjusting mobile Li ion concentrations approximate components found in LiPON films. In the simulated structures, we find that N is energetically more stable at bridging bond sites than at tetrahedral sites by 2-3 eV and that the Li ion migration energies are 0.5–0.6 eV, similar to values measured in LiPON films.

¹Supported by NSF Grants DMR-0405456, 0427055, and 0705239.

2 N. J. Dudney, Interface 17:3, 44 (2008) and listed references.


**1:15PM Z10.00011 ABSTRACT HAS BEEN MOVED TO Z22.00011** —

**1:27PM Z10.00012 Systematic Size-Dependence of Electrical Resistivity Profiles in Bi$_{2}$Sb$_{0.1}$Crystals**¹, DONGXIA QU, J.G. CHECKELSKY, Department of Physics, Princeton University, Y.S. HOR, R.J. CAVA, Department of Chemistry, Princeton University, N.P. ONG, Department of Physics, Princeton University — Recently, Fu and Kane reported that surface states with odd-Z are composed of species with linear and branched chains, respectively. Both these and related structures derived from substituting O with N and adjusting mobile Li ion concentrations approximate components found in LiPON films. In the simulated structures, we find that N is energetically more stable at bridging bond sites than at tetrahedral sites by 2-3 eV and that the Li ion migration energies are 0.5–0.6 eV, similar to values measured in LiPON films.

¹Supported by NSF-MRSEC under Grant DMR-0819860.

**1:39PM Z10.00013 Low temperature C/T$^3$ peak in dipole disordered Bi$_{2}$Ti$_{2}$O$_{7}$** GAVIN LAWES, RON TACKETT, AMBESH DIXIT, Wayne State University, ART RAMIREZ, LGS Innovations, JIM O’BRIAN, Quantum Design, BRENT MELOT, RAM SESHAIDI, UC Santa Barbara — The presence of a low temperature peak in C/T$^3$ vs T, indicating excess entropy above the Debye contribution, is practically ubiquitous among both crystalline and amorphous materials. We present specific heat measurements on Bi$_{2}$Ti$_{2}$O$_{7}$, which is known to have incoherent ionic displacements leading to dipole disorder, and other related crystalline materials, including Bi$_{2}$NbInO$_{7}$, Bi$_{2}$Ti$_{2}$O$_{7}$, Y$_2$Ti$_2$O$_7$, and PbTiO$_3$, all of which exhibit excess low temperature entropy. We find that the C/T$^3$ peak for these samples agree roughly with a proposed scaling relation, with the peak temperature for Bi$_{2}$Ti$_{2}$O$_{7}$ among the lowest reported for any crystalline material. We discuss our results in the context of understanding the evolution of crystalline degrees of freedom to glassy degrees of freedom through our investigations of more complicated phosphate structures based on combinations of tetrahedral P–O bonds and bridging P=O–P bonds. For example, crystalline Li$_{1.2}$PO$_{1.5}$F$_x$N$_{1-x}$ and P$_2$O$_5$ are composed of phosphate structures with linear and branched chains, respectively. Both these and related structures derived from substituting O with N and adjusting mobile Li ion concentrations approximate components found in LiPON films. In the simulated structures, we find that N is energetically more stable at bridging bond sites than at tetrahedral sites by 2-3 eV and that the Li ion migration energies are 0.5–0.6 eV, similar to values measured in LiPON films.

2 Supported by NSF Grants DMR-0405456, 0427055, and 0705239.

3 N. J. Dudney, Interface 17:3, 44 (2008) and listed references.


**1:51PM Z10.00014 Understanding the Material Thermodynamics of Two-Step Solar Thermochemical Water-Splitting Cycles**¹, BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University Department of Materials Science and Engineering, SUNSHINE TO PETROL GRAND CHALLENGE AT SANDIA NATIONAL LABORATORIES TEAM — Metal oxide materials may be used in two-step solar thermochemical water-splitting cycles to renewably produce hydrogen: At high temperature, the oxide material is reduced, and at a lower temperature, the material re-oxidizes upon contact with water vapor producing hydrogen gas. Here, we present the first completely general analysis of the equilibrium thermodynamics of a two-step metal oxide water splitting cycle. We use density functional theory (DFT) and CALPHAD modeling, to assess many proposed oxide cycles. Using CALPHAD thermodynamic data, we survey a large number of oxide materials, including Bi$_{2}$NbInO$_{7}$, Bi$_{2}$Ti$_{2}$O$_{7}$, Y$_2$Ti$_2$O$_7$, and PbTiO$_3$, all of which exhibit excess low temperature entropy. We find that the C/T$^3$ peak for these samples agree roughly with a proposed scaling relation, with the peak temperature for Bi$_{2}$Ti$_{2}$O$_{7}$ among the lowest reported for any crystalline material. We discuss our results in the context of understanding the evolution of crystalline degrees of freedom to glassy degrees of freedom through our investigations of more complicated phosphate structures based on combinations of tetrahedral P–O bonds and bridging P=O–P bonds. For example, crystalline Li$_{1.2}$PO$_{1.5}$F$_x$N$_{1-x}$ and P$_2$O$_5$ are composed of phosphate structures with linear and branched chains, respectively. Both these and related structures derived from substituting O with N and adjusting mobile Li ion concentrations approximate components found in LiPON films. In the simulated structures, we find that N is energetically more stable at bridging bond sites than at tetrahedral sites by 2-3 eV and that the Li ion migration energies are 0.5–0.6 eV, similar to values measured in LiPON films.

¹The authors acknowledge support from the Sunshine to Petrol Grand Challenge at Sandia National Laboratories.

**2:03PM Z10.00015 Using High-Voltage Direct Current in Removing Coke from a Zeolite Catalyst Grain**¹, ABDULAZIZ ALJALAL, King Fahd University of Petroleum and Minerals — Zeolite catalysts are commonly used in petroleum refining processes. Over a period of time, these catalysts lose their activity due to gradual deposition of carbonaceous materials, called coke. The coke catalysts are usually reactivated by combusting the coke at elevated temperatures in presence of an oxygen-enriched gas. But the elevated temperatures cause damages to the structure of the catalyst which result in reduced activity. Normally, the catalyst is reactivated 3 or 4 times before it must be returned to the manufacturer for reclamation of the valuable platinum and/or rhodium content. This study is an attempt to come up with a new procedure to remove coke from a zeolite catalyst grain using high-voltage direct current. It is found that the process is self-terminated due to the loss of electrical conductivity of the grain. In addition, it is found that there an optimum current range for which up to 90% of the coke can be removed. Higher or lower currents result in much smaller removal of the coke.

¹The support of KFUPM is acknowledged.

**Friday, March 20, 2009 11:15AM - 2:27PM**

Session Z12 DCMP DMP: Phase Transitions at Surfaces 308
11:15 AM Z12.00001 A martensitic-like transition in a normal alkane, JEFFREY HUTTER, SHAILESH NENE, ERIC KARHU, ROBERTA FLEMMING, The University of Western Ontario — The normal alkanes, \( \text{C}_n \text{H}_{2n+2} \), with a structure consisting of a single chain, are the simplest hydrocarbons. These are an interesting class of material, both in terms of their intrinsic properties and the fact that many biological molecules contain hydrocarbon domains. Normal alkanes exhibit an unusual phase diagram with several solid phases, some of which—the “rotator phases”—are characterized by positional order without long-range orientational order. We have found a striking pattern of twinned, striped domains that occurs in thin layers the monolonic rotator RV phase of tricosane (\( \text{C}_{23}\text{H}_{48} \)). We have studied this structure, and its transitions to other phases, by X-ray diffraction, as well as by optical and atomic-force microscopy. Intriguingly, transitions between the RV phase and the RI orthorhombic phase lying at higher temperatures appear to be diffusionless, and preserve molecular-scale features even after multiple transitions between the phases. These properties are reminiscent of martensitic transformations, which are better-known in metal alloys, but occur here at convenient temperatures and with slow kinetics.

11:27 AM Z12.00002 Monolayer solids of short (perfluoro)alkanes on graphite, L.W. BRUCH, University of Wisconsin-Madison — Calculations are reported for the relative stability of monolayer solid lattices on graphite for \( \text{C}_n\text{H}_6, \text{C}_n\text{F}_8, \text{C}_n\text{F}_6, \) and \( \text{C}_n\text{F}_x \). Triangular, centered rectangular and two-sublattice herringbone lattices are treated. The calculations use all-atom (AA) models and are based on non-bonding interactions formulated for three dimensional dense phases of alkanes and perfluoroalkanes.

11:39 AM Z12.00003 Simulation of methane on Al(111), MAJID KARIMI, CARL LEBLOND, IUP, WAHYU SETYAWAN, STEFANO CURTAROLO, Duke University, RENEE DIEHL, Penn State University, DUKE UNIVERSITY COLLABORATION, PENN STATE UNIVERSITY COLLABORATION, IUP COLLABORATION — Classical many-body interatomic potentials for methane molecules interacting with Al(111) are developed using the embedded-atom method (EAM). The optimized EAM parameters for methane-Al(111) are obtained by fitting to the data generated from the first principles calculations. Adsorption of methane on the Al(111) substrate is studied using the Grand Canonical Monte-Carlo method. Adsorption isotherms are calculated at several temperatures near the triple point temperature of methane \( T_t = 90K \), and structural parameters obtained from the adsorbed density profiles. The structures and the thermodynamics of film growth are compared to methane adsorption on other metal surfaces, graphite and the d-Al-Co-Ni quasicrystal. This research is supported by NSF and ACS-PRF.

11:51 AM Z12.00004 Conformation-controlled networking of H-bonded assemblies on surfaces, M. ENACHE, M. MATENA, M. STOEHR, University of Basel, Switzerland, T.A. JUNG, Paul-Scherer-Institute, Switzerland, A. LLANES-PALLAS, D. BONIFAZI, Universita di Trieste, Italy — In order to prepare networks that could undergo phase transitions through a thermally-induced inversion of the molecular conformation leading to a variation of the intermolecular interactions, directional intermolecular forces can be regarded as promising candidates. In particular, H-bonding interactions will be exploited since their intermolecular interaction strength and geometry can be controlled by the number and arrangement of available H-bonding donor or acceptor moieties. We studied the 2D self-organization of a conjugated molecule bearing terminal 2,6-di(acylamino)pyridine moieties [1], which are well-known to form H-bonds, on a Ag(111) surface by STM. The hexagonal porous network, which is formed for room temperature deposition, is transformed into a close-packed rhombic pattern by a thermally induced trans-cis inversion of the terminal groups. This transformation can be explained by the fact that the system wants to minimize its energy: at the same time the free surface energy is minimized while the number of H-bonds per terminal group is doubled from two to four. [1] A. Llanes-Pallas et al., Angew. Chem. Int. Ed. 2008, 47, 7726

12:03 PM Z12.00005 IR enhancement and the surface potential of n-alkanethiol SAMs on GaAs(001), GREGORY M. MARSHALL, Department of Electrical and Computer Engineering, Université de Sherbrooke, Sherbrooke, CAN, GREGORY P. LOPINSKI, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, CAN, FARID BENSAEBA, Institute for Chemical Process and Environmental Technology, National Research Council of Canada, Ottawa, CAN, JAN J. DUBOWSKI, Department of Electrical and Computer Engineering, Université de Sherbrooke, Sherbrooke, CAN — n-Alkanethiol self-assembled monolayers (SAMs) were prepared on the GaAs(001) surface according to [1]. FTIR modal analysis of the CH\(_2\) stretching mode region (2800-3000 cm\(^{-1}\)) verified SAM structural coherence, revealed evidence of an assembly threshold and allowed the absorption coefficient of the SAM phase to be directly measured. A 6x enhancement factor was observed relative to coefficients derived from the ion and polycrystalline phases. This effect is reviewed in terms of the molecular order and is largely attributed to the chemical properties of the surface [2]. Confirmation is provided by Kelvin Probe measurement of the sheet dipole potential, interpreted in terms of the Cooperative Molecular Field Effect [3]. [1] McGuiness et al., J. Am. Chem. Soc. 128, 5231 (2006). [2] Marshall et al., submitted. [3] Cahen et al., Adv. Funct. Mater. 15, 1571 (2005).

12:15 PM Z12.00006 Faceting of Ru(1120) Surface: A Model System for Catalysis, QUANTONG SHEN, WENHUA CHEN, HAO WANG, ROBERT BARTYNSKI, Rutgers University, PROFESSOR ROBERT A. BARTYNSKI TEAM — We have studied NO\(_2\)-induced faceting of a Ru(1120) surface by means of low energy electron diffraction (LEED), scanning tunneling microscopy (STM), and Auger electron spectroscopy (AES). By annealing the sample at \( > 600 \) K in NO\(_2\) \(-10^{-8}\) Torr, the surface becomes fully faceted as revealed by LEED although it is rather smooth, with only two layers exposed. The faceted surface remains the same at NO\(_2\) exposure ranging from 20 L to 12000 L and is stable for substrate temperature \( T < 850 \) K. The STM results confirmed the LEED observations and showed that the faceted surface consists of sawtooth ridges along the [001] direction with typical dimensions of \( \sim 5 \) nm in width and \( > 100 \) nm in length. We have found that the faceted O/Ru surface is very active for NH\(_3\) decomposition to produce H\(_2\) with high selectivity to N\(_2\) at room temperature.

12:27 PM Z12.00007 Oxygen-induced nano-faceting of the Pd(112) surface, ALINA VLAD, ANDREAS STIERLE, Max Planck Institute for Metals Research, 70569 Stuttgart, Germany, RASMUS WESTERSTROEM, EDVIN LUNGDREN, Department of Synchrotron Radiation Research, Institute of Physics, University of Lund, SE-221 00 Lund, Sweden, HELMUT DOSCH, Max Planck Institute for Metals Research — Extensive efforts are currently made to understand the elementary steps in heterogeneous catalytic reactions, with the ultimate goal of designing more efficient catalysts. The structure of the catalytically active particles, as well as the temperature and the gas phase pressure, play a decisive role in the behavior of these systems. We studied the interaction of oxygen with the Pd(112) surface from ultrahigh vacuum to atmospheric oxygen pressures by means of in-situ surface x-ray diffraction, high resolution core level spectroscopy and scanning tunneling microscopy. The rearrangement of the stepped (112) surface into different type of facets was observed and is strongly dependent on the oxygen pressure. The transition from different adsorbed-oxygen phases to the bulk oxide was also followed as a function of the oxygen pressure.
12:39PM Z12.00008 ABSTRACT WITHDRAWN

12:51PM Z12.00009 Phase-field theory for phase transition dynamics of reconstructed semiconductor surfaces, BANG-GUI LIU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — We propose a natural two-speed model for the phase dynamics of Si(111) 7×7 phase transition to unreconstructed phase. Our simulated results show that a 7×7 island decays with its shape kept unchanged, and its area decay rate is a constant increasing with its initial area. LEEM experiments concerned are explained, which confirms that the dimer chains and corner holes are broken first, and then the stacking fault is remedied slowly. We also propose a phase-field-crystal model for the (2×1)-(1×1) phase transitions of Si(001) and Ge(001) surfaces. Simulated periodic arrays of dimerization is consistent with STM images. Calculated temperature dependence of the dimerization indicates that normal dimers and broken ones coexist between T_N and T_F, and a first-order phase transition takes place in between. This phase-field method is a reliable approach to phase dynamics of surface phase transitions. Phys. Rev. Lett. 100, 056103 (2008).

1:03PM Z12.00010 Investigation of Structural Phase Transitions on Wurtzite Gallium Nitride Surfaces, TIANJIAO CHEN, ABHIJIT CHINCHORE, YINGHAO LIU, KANGKANG WANG, WENZHI LIN, ARTHUR SMITH, Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, OH 45701 — Surface structures of wurtzite gallium nitride (w-GaN) have been investigated previously,[1][2] and it is well known that above 300K there exist order-disorder phase transitions. For N-polar w-GaN (000-1) at 300K, a family of surface reconstructions occurs, including 1×1, 3×3, 6×6, and c(6×12). Not much is known, however, about what happens to these structures as they are cooled below 300K. We have recently developed a new epitaxy/analysis system, including a sample stage which can be both heated and cooled. The N-polar w-GaN surfaces are prepared using rf N-plasma-assisted molecular beam epitaxy, and monitored in-situ using reflection high energy electron diffraction (RHEED). The approach is to monitor the [11-20] and [10-10] RHEED diffractions during cryogenic cooling, starting with the 1×1 or 3×3 structures. A critical issue to explore is the interrelationship between surface gallium concentration and structural deformation. This study may provide the missing link to new reconstructions of w-GaN recently observed using LT scanning tunneling microscopy.[3] This work is supported by NSF (Grant No. 0730257). [1] A. R. Smith et al., Phys. Rev. Lett. 79, 3934 (1997). [2] A. R. Smith et al., Surface Science 423, 70 (1999). [3] D. Acharya, S.-W. Hla et al., unpubished.

1:15PM Z12.00011 Magnetism of bulk CrO_2 and its (0001) surface: An ab initio study, SIQI SHI, Department of Physics, Center for Optoelectronics Materials and Devices, Zhejiang Sci-Tech University, ALEKSANDER WYSOCKI, KIRILL BELASHCHENKO, Department of Physics and Astronomy, University of Nebraska Lincoln — Magnetic properties of bulk CrO_2 and its (0001) surface are surface studied using the LSDA+U method. Magnetic energies are well fitted by the Heisenberg model and the Neel temperature is calculated using the quantum pair-cluster approximation. Very good agreement with experiment is found for the equilibrium volume, spectral density, local magnetic moment, band gap, and the Neel temperature. The stable (0001) surface is known to be terminated by a Cr semilayer [1], but its detailed structure is unknown. We identify two competing surface sites. The configurational surface Hamiltonian is constructed from supercells and the structural thermodynamics is studied. We find that in a wide range of temperatures about 1/3 of Cr atoms are below the oxygen layer and that there is a ordering phase transition from \sqrt{3} \times \sqrt{3} to 1 \times 1. Further, we find that (0001) surface has a unique feature of having an uncompensated magnetic moment that is not destroyed by surface roughness. This phenomenon makes CrO_2 a promising exchange bias application. [1] M. Bender, et. al. J. Phys. Condens. Matter 7, 5289 (1995).

1:27PM Z12.00012 Fingerprint of surface magnetism in CrO_3 based exchange bias heterostructures, XI HE, YI WANG, CH. BINEK, University of Nebraska-Lincoln — Magnetolectric (ME) compounds have a recent revival as promising components of novel spintronic devices [1, 2, 3]. Since the magnetoelastic (ME) effect is relativistically small in traditional antiferromagnetic (AF) compounds like CrO_2 (max. αzz ≈ 4ps/m) and also cross-coupling between ferroic order parameters is typically small in the modern multiferroics, it is a challenge to electrically induce sufficient magnetization required for the envisioned device applications. In exchange bias systems the bias field depends critically on the AF interface magnetization. Hence, a strong relation between the latter and the surface magnetization of the free CrO_2 layer can be expected. Our recent research indicates that there are two magnetic phase transitions in free CrO_2 films accompanying surface structural phase transitions. Well defined AF interface magnetization is initialized through ME annealing to T=20K. Subsequently, the interface magnetization is thermally driven through phase transitions at T=120 and 210K. Their effects on the exchange bias are studied in CrO_2 (111)/CoPt films with the help of polar Kerr and SQUID magnetometry. [1] P. Borisov et al. Phys. Rev. Lett. 94, 117203 (2005). [2] Ch. Binek, B.Doudin, J. Phys. Condens. Matter 17, L39 (2005). [3] R. Ramesh et al. 2007 Nature Materials 6 21. Financial support by NSF through Career DMR-0547887, MRSEC DMR-0820521 and the NRI.

1:39PM Z12.00013 Magnetic Susceptibility χ of O_2 in Confined Geometries, TIMOTHY PRISK, PAUL SOKOL, Indiana University Cyclotron Facility — Bulk solid oxygen exhibits three distinct crystallographic and paramagnetic phases, α, β, γ (in order of ascending temperature). The thermodynamic behavior of some systems, including their possible phases and phase transition temperatures, are known to change in interesting and nontrivial ways as these systems are subjected to confined geometries. Recent work by Kilburn and Sokol on the phonon density of states for confined solid oxygen indicates that the first of these crystallographic phases, α, is completely suppressed. The magnetic susceptibility χ of solid oxygen confined within various porous materials will be presented. The effect of confinement on the magnitude of the susceptibility χ and the transition temperatures will be discussed.

This work was supported by the U.S. Department of Commerce, under Grant 70NANB5H1163.

1:51PM Z12.00014 Size dependent transport of amorphous Indium Oxide films, SWATI SOMAN, DAN SHAHAR, Weizmann Institute of Science, Israel. — Superconductivity in presence of disorder is a topic of interest among experimentalists as well as theoreticians for past several decades. Experiments performed on disordered films of various materials, elemental as well as mixture, have demonstrated Superconductor to Insulator transition (SIT) with increase in disorder or externally applied magnetic field. Disorder is difficult to quantify. However, in an experiment it is controlled by tuning film thickness and/or composition. We present experimental evidence of SIT, in disordered, amorphous Indium Oxide (aInO_x) films, which is tuned by films’ lateral dimensions. By fabricating films of same thickness and composition in Hall bar geometry and changing only the sizes of Hall bars, we observe that the sheet resistance per square, R changes with the size of the square, contrary to its definition. The systematic dependence of R on square size is observed to occur only for a critical disorder, similar to percolation model. The observations suggest an inhomogeneous nature of transport near SIT in our samples which are found to be structurally homogeneous. We postulate that such size dependent transport properties are possible to observe in disordered films of other materials that exhibit SIT.
2:03PM Z12.00015 Impact of Boron Additions on the A1 to L1₀ Phase Transformation in FePt Alloy Films. B. WANG, K. BARMAK, Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213 — The combination of high magnetocrystalline anisotropy energy density and good corrosion resistance has resulted in significant interest in L1₀ ordered alloys such as FePt for ultrahigh density, heat assisted magnetic recording (HAMR) media, with areal storage densities of ≥1Tb/in². When deposited at room temperature, these FePt forms in the chemically-disordered A1 state, requiring a post-deposition anneal to form the ordered L1₀ phase. Previous work has shown that the composition of FePt films has a significant impact on the kinetics and thermodynamics of the A1 to L1₀ phase transformation. In this paper, we report on the impact of ternary additions of B to FePt on the thermodynamic and kinetic parameters of the transformation. We also compare and contrast the impact of B additions with those of ternary additions of Cu and Ni. It is shown that the introduction of B into Pt-rich FePt films lowers the activation energy and the kinetic ordering temperature for the A1 to L1₀ phase transformation. However, this impact becomes negligible when B is introduced into Fe-rich FePt films.

2:15PM Z12.00016 ABSTRACT WITHDRAWN —

Friday, March 20, 2009 11:15AM - 1:15PM —
Session Z14 DFD: Equilibrium Self-Assembly

11:15AM Z14.00001 Para-, ferro- and antiferro-magnetic order in beta-sheet tapes of oligopeptides. SARA JABBARI-FAROUJII, PAUL VAN DER SCHOOT, Eindhoven University of Technology — Beta-sheet-forming peptides give rise to self-assembled hierarchical structures such as tapes, ribbons and fibrils, which at sufficiently high concentrations form nematic liquid crystalline solutions and gels. Applications of these novel materials are found in nanotechnology, medicine and personal care products. Such aggregates not only appear in the context of desirable biomaterials but also in pathological self-assembly of mis-folded proteins, forming aggregates such as “amyloids”. Recently a theoretical model was developed to understand the properties of these self-assembling structures [1]. The question which arises is what happens if we mix different peptide species varying e.g. in length or interaction energy. Do they mix in self-assembled structures or form separate ones? This is of crucial importance as most of industrially produced materials are not monodisperse. To model the simplest polydisperse system, we apply two-component self-assembled Ising model, in which three energy contributions play a role, depending on the relative values of these energy scales and concentrations of the two components, different morphologies of tapes consisting of both components are formed exhibiting paramagnetic, ferromagnetic or antiferromagnetic order. [1] A. Aggeli, et al; PNAS 2001, 98, 11857

11:27AM Z14.00002 Self-assembly induced protein crystallization. HONGJUN LIU, SANAT KUMAR, Columbia University, JACK DOUGLAS, NIST — The strongly anisotropic nature of inter-protein interactions naturally leads them to self-assemble into structures mirroring the symmetry of the inter-protein potential. Self-assembly is a thermodynamically distinct phenomenon from phase separation, and we consider whether it can play a direct role in nucleating protein crystals. Previous simulations and measurements have established that protein clusters formed below the critical point for liquid-liquid phase separation (Tc) can facilitate crystal nucleation. However, recent experiments have indicated the existence of clustering-induced protein nucleation even for T > Tc, where phase separation does not exist. Here we simulate a minimal model of patchy particles and indeed find that transient clusters formed through self-assembly (even above Tc) can nucleate crystal growth. Importantly, the self-assembled clusters help to select the symmetry of the resulting crystal growth. In contrast, protein crystallization for T < Tc does not have this directing influence, and polycrystalline growth forms, such as spherulites, are then prevalent. Our simulations suggest that self-assembly directed crystallization might be common in protein solutions and that this process is relevant for understanding protein crystallization polymorphism.

11:39AM Z14.00003 Mechanisms for semi-flexible filament self-assembly: an experimental and simulation study. LAM NGUYEN, Center for Materials Research and Technology (MARTECH), Department of Physics, Florida State University, WEI YANG, STEVE ACQUAH, HAROLD KROTO, Department of Chemistry & Biochemistry, Florida State University, LINDA HIRST, School of Natural Sciences, University of California, Merced — The self-assembly of semi-flexible filaments, such as F-actin, in the presence of cross-linkers has been studied experimentally and via molecular dynamics simulation. Several imaging techniques including fluorescence and electron microscopy have been used to elucidate the structural properties of formed bundles and networks of filaments. With the help of simulation we are able to observe the dynamical process of the self-assembly and study the driving forces behind filament aggregation. The roles of different parameters such as cross-linker density and filament length have been investigated, determining the assembled system properties. We find both of these parameters to play a key role in the final structure formation. Understanding the mechanism for the self-assembly of these semi-flexible filaments will be very useful in the application of developing a new class of biological materials.

1This research is supported by MARTECH at Florida State University and by the National Science Foundation Biomaterials Program (DMR-0745786).

12:03PM Z14.00005 Reversible pH-Induced Structural Transition in a Polyelectrolyte-Surfactant System: from Semi-flexible Rod to String of Spheres. VIET LAM, LYNN WALKER, Carnegie Mellon University — We have characterized a polyelectrolyte-surfactant system that forms stable rod-like aggregates in aqueous solution. While this structure is stable to most changes in solution condition, we have observed a reversible change in behavior with pH. This is due to a pH-induced structural transition from the original semi-flexible rod at neutral pH to a more flexible object at acidic conditions. A simple model of polyelectrolyte chain crossing multiple surfactant spherical micelles, or a string of spheres, has been proposed as the structure of the aggregates at low pH. This represents a novel rod-like nanoscale system that goes through a reversible gelation with pH, with possible use in oil drilling (matrix acidification aid), liquid flow control, or transport of hydrophobic materials. Here, we will present a simple model of the structural change and experimental justification.
12:15PM Z14.00006 Self-Assembly of Highly Segregating Diblock Copolymer in Solution, DILRU RATNAWEERA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHIA, Clemson University — Solvent affinity drives the association of diblock co-polymers in selective solvents. The shape of the micelles is affected by the size of the blocks and their interaction with the solvent. Most experimental and theoretical studies have investigated solutions of diblocks with a relatively low incompatibility, requiring relatively large blocks to associate. The current work introduces a small angle neutron scattering study of a highly segregated diblock-copolymer, a trifluoro propylmethyl siloxane - polystyrene (PTFPMS-PS) in toluene, a good solvent for the polystyrene. Studies were carried out over volume fractions of 0.1 to 0.5 of the fluorinated siloxane segment. The high degree of segregation results in association into star-like micelles with the fluorinated siloxane in the core and a swollen corona even at very low volume fractions of the fluorinated segments. The micelles exhibit unique temperature stability in comparison with aggregates formed by diblock-copolymers in a lower segregation regime. The detailed structure of these aggregates as a function of volume fraction and temperature will be discussed.

12:27PM Z14.00007 Mesophases of soft-sphere aggregates, HOMIN SHIN, GREGORY GRASON, CHRISTIAN SANTANGELO, University of Massachusetts, Amherst — Soft spheres interacting via a hard core and purely repulsive shoulder self-assemble into clusters forming a variety of mesophases. We combine a mean field theory developed from a lattice model with a level surface analysis of the periodic structures of soft-sphere aggregates to study stable morphologies for a class of interaction potentials. The mean-field solution shows that the site occupation densities and interparticle potential are self-consistently related to an “effective field” acting on each particle. In the strong segregation limit, the space group symmetry of possible aggregate structures associated with the spatially modulated field, together with a half-filling condition at the interface of morphology, allows us to produce a phase diagram including Lamella, Hexagonal-columnar, and BCC phases, and their inverse phases in the parameter space of chemical potential and interparticle potential. Finally, we discuss the finite-temperature corrections to strong segregation theory in terms of Sommerfeld-like expansion and how these corrections affect the thermodynamic stability of bicontinuous mesophase structures, such as gyroid.

12:39PM Z14.00008 Breaking it up: Simulations of micelle fission in explicit solvent, MIKKO KARTTUNEN, The University of Western Ontario, MARIA SAMMALKORPI, MIKKO HAATAJA, Princeton University — We study self-assembly in micellar systems consisting of sodium dodecyl sulfate (SDS) using detailed 200-400 ns atomic scale molecular dynamics simulations. The simulations were done with explicit solvent, counterions and salt. We focus on the role of molecular level interactions driving self-assembly [1] and, in particular, show how micelle fission can be controlled using electrostatics. As our main result, we demonstrate the existence of a new fission pathway in charged micelles [2] and provide a physical explanation for it.

12:51PM Z14.00009 Neutron Scattering Analysis of the Dynamics and Structure of Semi-flexible, Self-Assembled Peptide Chain Networks and WormLike Micelles, N. WAGNER, M. BRANCO, D.POCHAN, J. SCHNEIDER, University of Delaware — Self-assembled peptide hydrogels are formed from synthetic β-hairpin peptides that undergo triggered self-assembly to form a physically crosslinked network of entangled fibrils. Upon salt addition at pH 7.4, these peptides fold into a β-hairpin self-assembly to form a rigid hydrogel stabilized by non-covalent crosslinks. A single amino acid substitution is performed to charge the peptide and greatly alter the rate of assembly. As a result, faster folding and self assembly kinetics are observed leading to more rigid gels. Transmission electron microscopy (TEM) and rheology demonstrate that the resultant, rigid networks of the semiflexible fibrils are composed of a bilayer of hairpins with a cross-sectional diameter of 3 nm, corresponding to the width of a folded peptide. Neutron spin echo (NSE) measurements show that the peptides can be modeled as semiflexible chains on length scales shorter than the characteristic chain size. The chain diffusivity is reduced by the peptide substitution and this can be attributed to alteration of the electrostatic interactions between peptides in the fibril. Small angle neutron scattering (SANS) measurements show a transition from a cylindrical rod-like geometry to a more branched, fractal-like network topology upon amino acid substitution. These measurements explain the large increase in gel modulus observed upon amino acid substitution. These results facilitate the rational design of self-assembling peptide materials for biomaterial applications. NSE results for semiflexible wormlike micelles will also be discussed.

1:03PM Z14.00010 Chiral Self-Assembly of Rodlike Viruses, EDWARD BARRY, ZVONIMIR DOGIC, ROBERT MEYER, Brandeis University, ROBERT PELCOVITS, Brown University, RUDOLF OLDENBOURG, Marine Biological Laboratory — The self-assembly of two dimensional achiral membranes which occurs in entropic mixtures of monodisperse colloidal rods and non-adsorbing polymers will be described. The colloidal nature of the rod/polymer model system enables us to simultaneously examine the behavior of self-assembled membranes at both the molecular and continuum lengthscales. Combining observations made at the very different lengthscales, we investigate how chirality frustrates assembly of achiral 2D membranes altogether, and instead drives the formation of very complex and highly regular chiral structures. Representative structures obtained through chiral self-assembly include: twisted ribbons, double helices, two dimensional analogs of a TGB phase, and regular arrays of pores embedded within a 2D membrane.

Friday, March 20, 2009 11:15AM - 2:15PM –
Session Z16 DAMOP: Bosons in Optical Lattices II

11:15AM Z16.00001 Optical lattice-based addressing and control of long-lived neutral-atom qubits, NATHAN LUNDBLAD, TREY PORTO, IAN SPIELMAN, RADU CHICIREANU, WILLIAM PHILLIPS, QJI/NIST/UMD — Many proposed quantum computational platforms are driven by competing needs: isolating the quantum system from the environment to prevent decoherence, and easily and accurately controlling the system with external fields. For example, neutral-atom optical-lattice architectures provide environmental isolation through the use of states that are robust against fluctuating external fields, yet external fields are inherently useful for qubit addressing. Here we demonstrate a technique to address qubits formed from a pair of field-insensitive states by transferring the qubit into a different pair of field-insensitive states. A spatially inhomogeneous external field allows the addressing of particular “marked” elements of a qubit register, leaving unmarked qubits unaffected, despite the presence of crosstalk or leakage of the addressing field. We demonstrate this technique in an ensemble of $^{87}$Rb atoms and show that we can robustly perform single-qubit rotations on qubits located at addressed lattice sites. This precise coherent control is an important step forward for lattice-based neutral-atom quantum computation, and is applicable to state transfer and qubit isolation in other architectures using field-insensitive qubits.

11:27AM Z16.00002 ABSTRACT WITHDRAWN –
11:39AM Z16.00003 Vortices near the Mott phase of a trapped Bose-Einstein condensate\textsuperscript{1}, DANIEL GOLDBAUM, ERICH MUELLER, Cornell University — We present a theoretical study of vortices within a harmonically trapped Bose-Einstein condensate in a rotating optical lattice. We find that proximity to the Mott insulating state dramatically affects the vortex structures. To illustrate we give examples in which the vortices: (i) all sit at a fixed distance from the center of the trap, forming a ring, or (ii) coalesce at the center of the trap, forming a giant vortex. We model the imaging of these structures by calculating time-of-flight column densities. As in the absence of the optical lattice, the vortices are much more easily observed in a time-of-flight image than in-situ.


\textsuperscript{1}This material is based on work supported by the National Science Foundation through grant No. PHY-0758104

11:51AM Z16.00004 Boson Hubbard model with weakly coupled fermions\textsuperscript{1}, SUMANTA TEWARI, Department of Physics, Clemson University, Clemson, SC, ROMAN LUTCHYN, Condensed Matter Theory Center (CMTC) and Joint Quantum Institute (JQI), Department of Physics, University of Maryland, College Park, MD, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD — Using an imaginary-time path integral approach, we develop the perturbation theory suited to the boson Hubbard model, and apply it to calculate the effects of a dilute gas of spin-polarized fermions weakly interacting with the bosons. The full theory captures both the static and the dynamic effects of the fermions on the generic superfluid-insulator phase diagram. We find that, in a homogenous system described by a single-band boson Hubbard Hamiltonian, the intrinsic perturbative effect of the fermions is to suppress the Mott insulating lobes and enhance the superfluid phase.

\textsuperscript{1}Work supported by ARO-DARPA

12:03PM Z16.00005 Boson Hubbard model with weakly coupled fermions: Effects of higher bands and shrinking of the superfluid phase\textsuperscript{1}, SANKAR DAS SARMA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD, ROMAN LUTCHYN, Condensed Matter Theory Center (CMTC) and Joint Quantum Institute (JQI), University of Maryland, College Park, MD, SUMANTA TEWARI, Department of Physics, Clemson University, Clemson, SC — We study Boson Hubbard model with weakly coupled fermions and take into account the effects of the higher boson Bloch bands. For attractive couplings between the bosons and the fermions, mixing of the higher bands results in an effective enhancement of the boson on-site repulsion. The overall shift of the boson Hubbard phase diagram due to the presence of the fermions is thus determined by two competing effects: an effective fermion-mediated interaction between the constituent bosons (which favors the superfluid phase), and the renormalization of the boson-boson interaction due to the virtual boson transitions to the higher Bloch bands (which favors the Mott insulating phase). We find that the latter is typically dominant for the cold-atom experiments, which is consistent with the observed loss of the superfluid coherence in recent experiments.

\textsuperscript{1}Work supported by ARO-DARPA

12:15PM Z16.00006 Scattering Properties of Bose-Hubbard Hamiltonians with Two and Three Sites, MORITZ HILLER, STEFAN HU NN, Department of Physics, Albert Ludwigs University of Freiburg, Germany, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown CT-USA and MPI for Dynamics and Self-Organization, Göttingen-Germany, DORON COHEN, Department of Physics, Ben-Gurion University, Beer-Sheva, Israel, ANDREAS BUCHLEITNER, Department of Physics, Albert Ludwigs University of Freiburg, Germany — We consider a probe particle in a tight binding with two leads and a central site that is coupled to a Bose-Hubbard system consisting of two or three wells (dimer/trimer). In the case of the dimer we find that the resonance widths undergo a sequence of bifurcations resulting from the complexity of the underlying classical phase space structure. For the trimer we show that the statistical properties of the scattering matrix are well described by the random matrix theory predictions for chaotic scattering. The origin of this agreement is due to the fact that inelastic scattering from a chaotic system (trimer) is formally equivalent to elastic scattering in a waveguide that has a chaotic mode space.

12:27PM Z16.00007 Quantum fluctuations and self-organization of a BEC in a multimode optical cavity, SARANG GOPALAKRISHNAN, BENJAMIN LEV, PAUL GOLDBART, University of Illinois at Urbana-Champaign — An ultracold bosonic gas, trapped in an optical cavity, crystallizes at either the even or the odd antinodes of the cavity mode, if the cavity is pumped transversely with a strong laser beam. Spontaneous symmetry breaking between even and odd antinodes is favored because atoms spaced one wavelength apart coherently emit light absorbed from the laser, populate the cavity with photons, and thus trap themselves in attractive optical potential wells. For a single-mode cavity, the transition to a crystalline state has been observed \cite{1} and is well described by mean-field theory \cite{2}. However, in multimode cavities, either confocal or concentric, fluctuations are enhanced and change the character of the transition, resulting in a quantal version of the Brazovskii transition in layering systems. We derive a field-theoretic description of the atom-cavity system near the transition, and describe how fluctuations and defects imprint themselves on the correlations of the light leaking out of the cavity. \cite{1} A.T. Black et al, Phys. Rev. Lett. 91, 203001 (2003). \cite{2} J.K. Asboth et al, Phys. Rev. A 72, 053417 (2005).

12:39PM Z16.00008 Role of Spatial Inhomogeneity in the Experimental Determination of the Two Dimensional Bose-Hubbard Model Critical Point, KHAN W. MAHMUD, University of California, Davis, VALERY G. ROUSSEAU, Institut-Lorentz, LIÓN, Universiteit Leiden, Postbus 9504, 2300 RA Leiden, The Netherlands, MARCOS RIGOL, Georgetown University, GEORGE G. BATROUNI, University of Nice, RICHARD T. SCALETTER, University of California, Davis — Recent experiments at NIST on confined Rb atoms in two dimensions, combined with high precision Quantum Monte Carlo (QMC) values for the homogeneous Bose-Hubbard model critical point, represented important progress toward testing the concept of optical lattice emulator. The experimentally determined critical coupling for the superfluid-Mott transition is in quite good agreement with the QMC results \(U/J_0 = 16.74\) for the homogeneous case. We present an analysis of these results which takes into account the spatial inhomogeneity arising from the confining potential. We perform a detailed QMC calculation of the density profile, local density fluctuations, and condensate fraction along the trajectory followed experimentally. We demonstrate how the number of atoms, optical lattice depth, curvature of the confining potential, and temperature in the NIST experiment, the critical value for the formation of Mott domains is rather close to that of the homogeneous system.

12:51PM Z16.00009 Superfluid to Mott-insulator transition of hardcore bosons in a superlattice, ITAY HEN, MARCOS RIGOL, Georgetown University — We present results of analytical and numerical studies of the superfluid to Mott-insulator transition of hardcore bosons in a superlattice potential in arbitrary dimensions. In this study, we use mean-field plus spin-wave corrections and the stochastic series expansion (SSE) algorithm to compute various properties of the system, such as the ground-state energy, the condensate fraction, the superfluid density, and the compressibility. We will show that in some cases the spin-wave approximation is in remarkable agreement with the exact numerical results.
1:03PM Z16.00010 The single-atom box: bosonic staircase and effects of parity, CHRISTOPH BRUDER, Department of Physics, University of Basel, 4056 Basel, Switzerland, D.V. AVERIN, T. BERGEMAN, Department of Physics and Astronomy, SUNY, Stony Brook, NY 11794-3800 University of Stony Brook, P.R. HOSUR, Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — We have developed [1] a theory of a Josephson junction formed by two tunnel-coupled Bose-Einstein condensates in a double-well potential in the regime of strong atom-atom interaction for an arbitrary total number \( N \) of bosons in the condensates. The tunnel resonances in the junction are shown to be periodically spaced by the interaction energy, forming a single-atom staircase sensitive to the parity of \( N \) even for large \( N \). One of the manifestations of the staircase structure is the periodic modulation with the bias energy of the visibility of the interference pattern in lattices of junctions. A different, e.g. fermionic, additional particle in the junction leads to non-trivial modifications of the staircase, that can be experimentally observed in the visibility of the interference pattern. [1] D.V. Averin, T. Bergeman, P.R. Hosur, and C. Bruder, Phys. Rev. A 78, 031601(R) (2008).

1:15PM Z16.00011 Spin field effect transistors with ultracold atoms\(^1\) , G. JUZELIUNAS, J. RUSECKAS, Institute of Theoretical Physics and Astronomy of Vilnius University, CHARLES W. CLARK, J.Y. VAISHNAV, Joint Quantum Institute, National Institute of Standards and Technology — We propose a method of constructing cold atom analogs of the spintronic device known as the Datta-Das transistor (DDT), which despite its seminal conceptual role in spintronics, has never been successfully realized with electrons. We propose two alternative schemes for an atomic DDT, both of which are based on the experimental setup for tripod stimulated Raman adiabatic passage. Both setups involve atomic beams incident on a series of laser fields mimicking the relativistic spin orbit coupling for electrons that is the operating mechanism of the DDT.


1:27PM Z16.00012 Vortex quantum dynamics of two dimensional lattice bosons, NETANEL LINDNER, ASSA AUERBACH, Physics Department, Technion, Israel, DANIEL P. AROVAS, University of California at San Diego — We study hard core lattice bosons in a magnetic field near half filling\(^2\). The strong periodic potential scatters the vortices by units of reciprocal lattice momenta, enhancing their mobility and modifying their effective Magnus field. The bare vortex hopping rate on the dual lattice is extracted by exact diagonalizations of square clusters. We deduce quantum melting of the vortex lattice above vortex density of \( 6.5 \times 10^{-3} \) per lattice site. The Hall conductivity, which reflects the vortex Magnus dynamics, reverses sign abruptly at half filling. The characteristic temperature scale of the Hall conductivity vanishes at the transition point. We prove that at half filling, each vortex carries a spin half quantum number ('v-spin'). Experimental implications of these results are relevant for diverse systems of current interest, e.g. cold atoms on rotating optical lattices, arrays of Josephson junctions and underdoped cuprate superconductors.

\(^2\) See: arXiV:0810.2604

1:39PM Z16.00013 Mapping out the finite temperature phase diagram of the Bose-Hubbard model\(^3\), QI ZHOU, Department of Physics, The Ohio State University, YASUYUKI KATO, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo, QI ZHOU, Department of Physics, The Ohio State University, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo — We propose a method to experimentally map out the phase diagram of Bose-Hubbard Model at finite temperatures solely based on the density distribution of trapped bosonic atoms in optical lattices. Based on Quantum Monte Carlo simulations in a trap with 10\(^5\) bosons, we show that the phase boundary between the superfluid and normal state is directly located from kinks in the compressibility, which are extracted from the density profile itself. The temperature of bosons in the lattice is obtained from the density profile at the edge. Our method uses general aspects of critical fluctuations at a phase transition and can be extended to other systems, even when exact numerical simulations are not available.

\(^3\) NT acknowledges support from ARO and DARPA under grant # W911NF-08-1-0338.

1:51PM Z16.00014 Distributions of entropy and superfluid density of trapped bosons in optical lattices\(^4\), NANDINI TRIVEDI, Department of Physics, The Ohio State University, YASUYUKI KATO, Institute for Solid State Physics, University of Tokyo, QI ZHOU, Department of Physics, The Ohio State University, NAOKI KAWASHIMA, Institute for Solid State Physics, University of Tokyo — Based on a large scale quantum Monte Carlo simulations of the Bose Hubbard model using the worm algorithm\(^1\), we calculate the inhomogeneous distribution of entropy and superfluid density of trapped bosons in optical lattices. We show that most of the entropy is concentrated in the conducting shells. As the lattice is ramped up under adiabatic conditions, we show that the temperature increases and the superfluid regions in the trap can vanish. However, by opening up the trap at fixed lattice height, the system effectively cools, the entropy gets redistributed in the trap and superfluid regions reemerge. [1] Sharp Peaks in the Momentum Distribution of Bosons in Optical Lattices in Normal State Yasuyuki Kato, Qi Zhou, Naoki Kawashima and Randini Trivedi Nature Physics, 4, 617 (2008)

\(^4\) NT acknowledges support from ARO and DARPA under grant # W911NF-08-1-0338.

2:03PM Z16.00015 Observing the Quantum Spin Hall Effect with Ultracold Atoms, J.Y. VAISHNAV, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg MD 20899, TUDOR D. STANESCU, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, CHARLES W. CLARK, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg MD 20899, VICTOR GALITSKI, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742 — The quantum spin Hall (QSH) state is a topologically nontrivial state of matter proposed to exist in certain 2-D systems with spin-orbit coupling. While the electronic states of a QSH insulator are gapped in the bulk, a QSH insulator is characterized by gapless edge states of different spins which counterpropagate at a given edge; the spin is correlated with the direction of propagation. Recent proposals\(^5\) suggest that synthetic spin-orbit couplings can be created for cold atoms moving in spatially varying light fields. Here, we identify an optical lattice setup which generates an effective QSH effect for cold, multilevel atoms. We also discuss methods for experimental detection of the atomic QSH effect.


Friday, March 20, 2009 11:15AM - 12:51PM –
Session Z17 GQI: Spin Qubit Coherence and Control 318

11:15AM Z17.00001 ABSTRACT WITHDRAWN
Pulse of light from a molecular system appears as a result of enhanced spontaneous emission rate due to interactions via the electromagnetic field. Consequently, their wavelength can be similar to that of the sample size. This is the elementary condition for Dicke's super-radiance. In this radiative process a short intense

Institute of Technology, Haifa 32000, Israel — Photons emitted by transition between the discrete levels of single molecular magnets have an interesting property:

AMIT KEREN, Department of Physics, Technion - Israel Institute of Technology, Haifa 32000, Israel, OREN SHAFIR, Physics Department, Technion-Israel Institute of Technology, Haifa 32000, Israel. Supported by the U.S. Department of Energy, Materials Science Division under contract No. DE-AC05-00OR22725 with Oak Ridge National Laboratory and operated by UT-Battelle, LLC, and the National Science Foundation under grant DMR-0412231.

...atoms in "contact" with the substrate plane, while the benzene is more planar. These studies will be compared to results of neutron scattering investigations.

...rotational motion has a distinct out of plane component coupled to the translational diffusion much like the rolling motion of a wobbly wheel with three hydrogen...

...for the electron-spin-resonance (ESR) measurements in a spin-1/2 Heisenberg anti-ferromagnetic spin chain. At the non-interacting level, a non-orthogonal orientation of the magnetic field and DM vector leads to a sharp delta-function ESR signal for the right and left moving excitations. The peak positions and their...

...the relevant parameter regimes and clarify the importance of this decoherence effect.

1 This work is supported by NSA/LPS through ARO, and NSF.

11:39AM Z17.00003 Soft-pulse refocusing in the presence of Markovian dephasing. GREGORY D. QUIROZ, USC, LEONID P. PRYADKO, UCR — We consider the effect of Markovian decoherence on the performance of refocusing sequences. This is relevant if dynamical coupling is to be concatenated with quantum error correcting codes as the first stage of decoherence protection. The basic effect is that an asymmetric decoherence can cause a change in the direction of polarization of a quantum system. For example, dephasing of a single qubit reduces transverse components of the spin polarization vector, thus shifting it towards the z axis. In this work we construct perturbation expansions of effective decoherence operators for generic shaped pulses, and for several sequences of π and π/2-pulses. While in general the performance of soft pulses is worse that that of the ideal δ-pulses, the detrimental effect of dephasing can be reduced by pulse shaping.

11:51AM Z17.00004 Fock-Space Coherence in Quantum Dots. EDUARDO VAZ, JORDAN KYRIAKIDIS, Dalhousie University — We investigate the non-Markovian time evolution of the Fock-space coherence between states with different particle numbers in a multilevel quantum dot. By analyzing the off diagonal density matrix elements for a model for which the dominant relaxation mechanism is through sequential tunneling transport, we observe a decoupling between the evolution of the Fock-space coherence and that of the population probabilities for the dot states. When tunneling rates to distinct orbitals differ — a common occurrence — the decoherence time of the Fock-space elements of the density matrix can be dramatically increased even when the Hilbert-space coherence between states with particle number decreases. This is an example of how a many-body coherence can remain robust even in the presence of rather large single-particle noise.

12:03PM Z17.00005 Randomized Benchmarking of Superconducting Qubits. JERRY M. CHOW, Yale University, JAY GAMBITTA, University of Waterloo, LARS TORNBERG, Chalmers University, JENS KOCH, LEV BISHOP, ANDREW HOUCIK, STEVEN GIVIN, Yale University, ROBERT SCHÖLEKOPF, YALE CIRCUIT QED TEAM — We present measurements of average gate errors for a superconducting qubit using randomized benchmarking [1]. The results are compared with gate errors obtained from a double π pulse experiment and quantum process tomography. Randomized benchmarking reveals a minimum average gate error of 1.1 ± 0.3% and a simple exponential dependence of fidelity on the number of applied gates. It shows that the limits on gate fidelity are primarily imposed by qubit decoherence and finite gate lengths (constrained by qubit anharmonicity), in agreement with theory.


12:15PM Z17.00006 Simulating quantum spin systems with superconducting electrical circuits. EMILY PRITCHETT, MICHAEL GELLER, University of Georgia — There is currently great interest in the simulation of quantum spin and lattice models using cold atoms. Motivated by experimental progress in the fabrication and control of superconducting electrical circuits and their use in quantum information processing, we investigate their use as simulators of quantum spin systems, and consider a wide family of spin models that can be simulated with existing Josephson junction devices.

12:27PM Z17.00007 Electromagnetic radiation emanating from the molecular nanomagnet Fe₈. AMIT KEREN, Department of Physics, Technion - Israel Institute of Technology, Haifa 32000, Israel, OREN SHAFIR, Physics Department, Technion-Israel Institute of Technology, Haifa 32000, Israel. — Photons emitted by transition between the discrete levels of single molecular magnets have an interesting property: their wave length can be similar to that of the sample size. This is the elementary condition for Dicke's super-radiance. In this radiative process a short intense pulse of light from a molecular system appears as a result of enhanced spontaneous emission rate due to interactions via the electromagnetic field. Conversely, several investigators have been looking for this type of radiation in the molecular magnet Mn₁₂, where energy bursts were reported after magnetic avalanches. We investigate the same phenomenon in the Fe₈ molecule. Unlike in Mn₁₂, we found energy bursts each time there is a jump in the magnetization, confirming their quantum nature. A series of tests indicated that photons carry out the energy. These photons obey the elementary conditions for super-radiance.

12:39PM Z17.00008 Asymmetries in electron spin resonance signal of magnetized spin chains and quantum wires due to spin-orbital interactions. SUHAS GANGADHARAAIHAV, University of California, Irvine, OLEG STARYKH, University of Utah, Salt Lake City — We discuss consequences of the symmetry breaking Zeeman and uniform Dzyaloshinskii-Moriya (DM) terms for the electron-spin-resonance (ESR) measurements in a spin-1/2 Heisenberg anti-ferromagnetic spin chain. At the non-interacting level, a non-orthogonal orientation of the magnetic field and DM vector leads to a sharp delta-function ESR signal for the right and left moving excitations. The peak positions and their intensities generally differ, and can serve as a possible chiral probe for the two excitations. Similar results hold for a magnetized quantum wire with spin-orbit terms. Including a momentum dependent fluctuations in the spin-orbit coupling smears the delta-function and instead results in an asymmetric square root singularity. We discuss the role of temperature and interactions in the further modification of the ESR signal.

Friday, March 20, 2009 11:15AM - 2:15PM — Session Z18 DPOLY: Surfaces and Adsorption II 319

11:15AM Z18.00001 Dynamics of six-member molecular rings adsorbed onto graphite and MgO(100). JOHN Z. LARESE, Oak Ridge National Laboratory and University of Tennessee, PETER YARON, University of Tennessee — Molecular dynamic studies of adsorption of six-member molecular rings (cyclohexane and benzene) onto various substrates (like MgO(100) and graphite) have been undertaken using a commercial modeling package (Materials Studio by Accelrys Software Inc.) that employs central force field potentials. These studies indicate that both systems exhibit rotational translational coupling and strong signs that the translational diffusion is lattice-like on graphite. The cyclohexane rotational motion has a distinct out of plane component coupled to the translational diffusion much like the rolling motion of a wobbly wheel with three hydrogen atoms in “contact” with the substrate plane, while the benzene is more planar. These studies will be compared to results of neutron scattering investigations of the temperature dependence of the dynamics.

1 Supported by the U.S. Department of Energy, Materials Science Division under contract No. DE-AC05-00OR22725 with Oak Ridge National Laboratory and operated by UT-Battelle, LLC, and the National Science Foundation under grant DMR-0412231.
The scaling parameter has no universal value but depends on the molecular length. C12, C24) of different lengths (7-30 ˚A) are scaled down by the use of the “scaling factor” (SF). Typically, this SF is assumed to be universal (and ∼ 0.5). In this talk, we study this universality hypothesis by comparing computational and experimental melting temperatures of alkane monolayers adsorbed on a solid graphite surface. In particular, melting of the bilayer is preceded by compression of the first layer, which has not been observed before. The results are compared with simulations of two similar systems: (i) three nitrogen layers confined in slit graphite pore, and (ii) an adsorbed incommensurate structure that mimics low temperature alpha phase of bulk nitrogen.

Surface Hopping and Sliding of Single DNA Chains under Electric Field, BENXIN JING, JIANG ZHAO, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — The motion of non-adsorbing DNA chains under electric field at solid-liquid interfaces was investigated by single molecule fluorescence microscopy at the total internal reflection geometry (TIRF). In-situ observation discovered that the motion of single non-adsorbing lambda-DNA chains was hopping-and-sliding-like along the surface. By varying the surface chemistry of the solid substrates, from the negative-charged hydroxyl group-rich surface to positive-charged amino group-rich surface, as well as hydrophobic surfaces, the dependence of DNA mobility on the surface-DNA interaction was studied. The results show that a well-defined dependence of the mobility of DNA on the surface polarity with respect to DNA itself. The study on different surfaces such as hydroxyl, amide, amino, and methyl-group rich surface show a sequence of DNA mobility of hydroxyl > amide> amino. The mobility of DNA on methyl terminated surface was found to be similar to that in amino surface.

First Principles study of the formation of molecular junctions: benzenethiolate on Au (111), YONGDUO LIU, VIDVUDS OZOLINS — We perform density functional calculations to study the formation mechanism of benzenethiolate molecular junctions on the Au (111) surface. Specifically, we investigate the geometry change and the mechanical properties of the molecular contact when it is under stretching. It is found that by pulling up the thiolate molecule from Au (111), one Au surface atom can be converted to an adatom. Moreover, if the stretching is continued, another Au atom would successively be pulled up to form a two-atom bridge between the Au (111) and the sulfur end group. Based on these findings, we propose a mechanism to the formation of pyramidal molecular junctions: benzenethiolate on Au (111).

Molecular Dynamics Simulation of friction in contact-mode Atomic Force Microscopy of alkane films and nanoparticles, F.Y. HANSEN, Tech. U. of Denmark, P. SOZA, P.U. Catolica Chile, H. TAUB, U. Mo-Columbia, U. VOLKMAN, P.U. Catolica Chile — In addition to sample topography, contact-mode Atomic Force Microscopy (AFM) can yield the lateral frictional force experienced by the AFM tip as it moves across a surface. This frictional force is measured by the torsional angle of the microscope’s cantilever arm, which, in the case of a surface composed of highly anisotropic alkane molecules, can depend on the molecular orientation. We have conducted molecular dynamics simulations of an AFM tip moving over films and nanoparticles of C14H30 (C24) in the contact mode. For films in which the long axis of the C24 molecules is oriented parallel to the surface, we find a smaller frictional force in a scan direction perpendicular to the long axis than parallel to it. On surfaces where the alkane molecules are oriented perpendicular to the interface, we find that in all scan directions the frictional force is less than when the long molecular axis is parallel to the interface. All of these findings are consistent with experimental observations.

Support: U.S. NSF DMR-0705974 and FONDECYT 1060628 and 7070248


The Measurement of Surface Rheological and Surface Adhesive Properties of a PDMS Rubber using Micro- and Nano-Particle Embedment, STEPHEN HUTCHESON, GREGORY MCKENNA, Texas Tech University — In previous work, we used particle embedment data to determine the rheological response of the surfaces of a polystyrene film, a phase separated copolymer and a commercially available polydimethylsiloxane (PDMS) rubber through the application of a viscoelastic contact mechanics model. The goal of the current research is to build off this analysis and use micro- and nano-sphere embedment experiments to probe the surface rheological behavior of PDMS in the rubbery state. The work includes measurements made with different particle diameters and chemistries. An atomic force microscope (AFM) is used to measure the embedment depth as nanoparticles are pulled into the surface by the thermodynamic work of adhesion. Present results show that silica probes of different sizes (500 nm and 300 nm) give different results for the surface adhesion properties and the surface rheological properties determined from the particle embedment data and at scales much larger than the nanometer size scale where one might expect such deviations. Possible water entrapment and effects of particle surface composition on the results will be discussed.

Test of the universality of the scaling energy in alkanes based on the melting transition of monolayers adsorbed on graphite, L. FIRLEJ, Université Montpellier 2, B. KUCHTA, Université de Provence, M. ROTH, University of Northern Iowa, C. WEXLER, University of Missouri — The quality of the results of computational treatment of complex systems depends crucially on the quality of the interaction potentials used. When modeling non-rigid molecules an essential difficulty resides in the correct accounting for all energies related to internal degrees of freedom. Of particular importance is to avoid over- or under-counting non-bonded intramolecular van der Waals and electrostatic interactions between close neighbors that are chemically bonded. In many force fields (e.g. CHARMM) 1-4 non-bonded interactions are scaled down by the use of the “scaling factor” (SF). Typically, this SF is assumed to be universal (and ∼ 0.5). In this talk, we study this universality hypothesis by comparing computational and experimental melting temperatures of alkane monolayers adsorbed on a solid graphite surface. Three alkanes (C6, C12, C24) of different lengths (7-30 Å) have been analyzed using an all-atom representation, standard CHARMM parameters, and various SF’s. We show that the scaling parameter has no universal value but depends on the molecular length.

Support: U.S. DOE (DE-FG02-07ER46411), ACS-PRF (PRF42277-B5), and Univ. of Missouri Bioinformatics Consortium.
12:39PM Z18.00008 The role of local domain formation in the melting of hexane adlayers on graphite\textsuperscript{1}, M.W. ROTH, Univ. of Northern Iowa, L. FIRLEJ, B. KUCHTA, C. WEXLER, Univ. of Missouri — Hexane is the shortest alkane [CH$_3$-(CH$_2$)$_n$-CH$_3$] whose flexibility has any considerable impact on its dynamics. When adsorbed on graphite, a monolayer of hexane melts at a temperature of approximately 175 K. To understand the mechanisms of this transition we have performed large scale molecular dynamics simulations (several runs over 100 ns, total computation time ~ 10 cpu-years), using the most realistic model of the system (a fully atomistic representation of hexane, explicit site-by-site interaction with graphite carbons and CHARMM force field with carefully chosen adjustable parameters of interactions). We show that the melting of the low temperature herringbone solid phase starts with the formation of gauche defects at the ends of neighboring molecules, followed by molecular reorientation within a lamella, without perturbing the overall structure of the adsorbed film. The melted phase has a domain-type structure with domains’ orientation that reflects the 6-fold symmetry of graphite. The size of domains decreases progressively when the temperature increases and the deformation of molecules to quasi globular shape is driven by progressive formation of gauche defects.

\textsuperscript{1}Support: US-DOE (DE-FG02-07ER46411), ACS-PRF (PRF43277-B5), and Univ. of Missouri Bioinformatics Consortium.

12:51PM Z18.00009 Chain-length dependence in surface stresses of alkanethiolate-covered Au(111)\textsuperscript{1}, V. SRINIVASAN, Berkeley Nanoscience and Nanoengineering Institute, UC Berkeley, CA 94720, G. CICERO, Materials Science and Chemical Engineering Department, Politecnico di Torino, C.so Duca degli abruzzi 24, 10129, Torino, Italy, J. C. GROSSMAN, Berkeley Nanoscience and Nanoengineering Institute, UC Berkeley, CA 94720 — We have recently shown\textsuperscript{[1]} that adsorption-induced stresses in alkanethiolate-covered Au(111) contribute significantly to the stress-response in nano-mechanical cantilever sensors. In particular, we proposed a local stress relief (LSR) mechanism whereby charge removal by the Au-S bond from the Au surface promotes a stress reducing rearrangement of surface Au atoms. Since LSR depends on the nature of the Au-S bond it was unclear how the contribution to the stress- response would depend on the alkanethiolate structure. We present a first-principles study of the chain-length dependence in surface stresses of alkanethiolate-covered Au(111). We find that the surface stress upon adsorption is anisotropic and tensile, increasing in magnitude with the chain-length. We analyze this trend in the context of the LSR mechanism and inter-adsorbate interactions.

\textsuperscript{1}Supported by LDRD/Lawrence Livermore National Laboratory and UC Berkeley/NSF Grant No. 0425914

1:03PM Z18.00010 All-atom Molecular Dynamics simulations of partial pentane and hexane films on graphite\textsuperscript{1}, J. KASPAR, M.W. ROTH, University of Northern Iowa, CARLOS WEXLER, University of Missouri, L. FIRLEJ, Université Montpellier, B. KUCHTA, Université de Provence — We compare the self-assembly patterns of pentane (C$_{5}$H$_{12}$) and hexane (C$_{6}$H$_{14}$) adlayers physisorbed onto graphite at various coverages using the results of molecular dynamics simulations. Near monolayer coverage, the solid low temperature structure of the pentane film is nematic-like, and that of hexane-herringbone-like. At submonolayer coverages both systems exhibit three distinct topological regimes: vacancy patches in surface stresses of alkanethiolate-covered Au(111). We find that the surface stress upon adsorption is anisotropic and tensile, increasing in magnitude with the chain-length. We analyze this trend in the context of the LSR mechanism and inter-adsorbate interactions.

\textsuperscript{1}Work supported by the U.S. Department of Energy (DE-FG02-07ER46411) and the American Chemical Society Petroleum Research Fund (PRF43277-B5). Computational resources were provided by the University of Missouri Bioinformatics Consortium.

1:15PM Z18.00011 Temperature Dependent Adsorption Dynamics of Binary Mixtures of Halomethanes on Graphite and α-quartz Surfaces\textsuperscript{1}, JONATHAN NEHRING, North Park University, G. LEUTY, MESFIN TSIGE, Southern Illinois University at Carbondale — Using atomistic molecular dynamics simulations, we have investigated the structure and dynamics of binary mixtures of halomethanes (CF$_{3}$, CF$_{2}$Cl, and CF$_{2}$Br) as a function of temperature on two structurally and chemically different surfaces. The initial distribution of the binary mixture is either they are uniformly mixed or a layer or layers of one component is placed on top of a layer or layers of the other component. As a function of temperature (below and above the melting temperature of CF$_{3}$) and the two surface types, we observed a marked change on the concentration, dynamics, orientation, and structure of each of the components in the first layer of the binary mixtures next to the surfaces.

\textsuperscript{1}Work supported by the Donors of the American Chemical Society Petroleum Research Fund.

1:27PM Z18.00012 Liquid Chromatography at Critical Conditions: Balancing size exclusion and adsorption in nanopores\textsuperscript{1}, ASEM ABDULAHAD, JEFFREY AMOS, CHANG RYU, Rensselaer Polytechnic Institute — Liquid chromatography at critical condition (LCCC) is a measure to identify thermodynamic conditions, in which polymers elute independently of molar mass during high performance liquid chromatography. Under these critical conditions the entropic exclusions that dominate size exclusion chromatography (SEC) and the enthalpic adsorption that governs adsorption-based interaction chromatography (IC) are said to negate one another resulting in simultaneous elution of the polymer of different molecular weights. Using multiple C18-bonded silica columns with different average nanopore sizes (from 5 nm to 30 nm), we will study the LCCC conditions of PS in methylene chloride/acetone solvent mixture at different temperature. In addition, we will show that the separation of polystyrene can be fine tuned using a refined temperature gradient interaction chromatography (TGIC) that employs multiple columns of varying pore size in sequence.

\textsuperscript{1}This work is supported by the Nano / Bio Interface Center at the University of Pennsylvania and the U.S. National Science Foundation under grant number DMR-0425780.

1:39PM Z18.00013 Using Amphiphilic Copolymers and Nanoparticles to Organize Charged Biopolymers\textsuperscript{1}, JUNG HYUN PARK, MARLA MCCONNELL, YUJIE SUN, YALE GOLDMAN, RUSSELL COMPOSTO, University of Pennsylvania — Nanoparticles (NPs) on amphiphilic random copolymers control filamentous actin (F-actin) attachment. 3-aminopropyltriethoxysilane (APTES) coated silica NPs are selectively bonded to acrylic acid groups on the surface of a polystyrene-r-acrylic acid (PS-r-PAA) film. By changing the concentration of NPs in the medium, the surface density of positively charged anchors is tuned. Using total internal reflection fluorescence (TIRF) microscopy, immobilization of F-actin is observed via electrostatic interaction with NPs at high NP coverages. Below a critical coverage, F-actin is weakly attached and undergoes thermal fluctuations near the surface. Another method to tune F-actin attachment is to use APTES to cross-link and create positive charge in PAA films. Here, the surface coverage of F-actin decreases as APTES concentration increases. This observation is attributed to an increase in surface roughness and hydrophobicity that reduces the effective surface sites that attract F-actin. In addition, in-situ G-actin polymerization to F-actin is observed on both the NP and cross-linked PAA templates.

\textsuperscript{1}This work is supported by the Nano / Bio Interface Center at the University of Pennsylvania and the U.S. National Science Foundation under grant number DMR-0425780.
SCOTT MILNER, Penn State University — The conformation of polymer chains emerging from the face of a crystalline lamella has long been a matter of dispute. Long ago, arguments pitted “adjacent reentry” versus the “switchboard model” as extreme limits of possible behavior. Later, two theoretical approaches were attempted, but one (the Gambler’s Ruin model) did not properly account for the constraint of melt density, and the other (heuristic configuration counting of Flory et al.) did not account for chain connectivity. These shortcomings are resolved by a new “pseudobrush” theory of the amorphous interphase, which represents the reentrant chains as a polydisperse brush of loops in a self-consistent hydrostatic pressure field. This theory predicts the fraction of adjacent reentry, shows how the anisotropy of the interphase dies away with distance, and how the Gambler’s Ruin model is recovered far from the interface. Extension to the case of a finite slab between two crystal-melt interfaces predicts the frequency of tie chains, a key parameter for nonlinear deformation and ductile failure of semicrystalline polymers.

BERNARD LOTZ, Institut Charles Sadron, Strasbourg, INSTITUT CHARLES SADRON TEAM — The major structure and morphology features of polymer lamellae (and single crystals) are usually defined by the characteristics of the crystal lattice (cell geometry and symmetry, stem length). However, the fold surfaces that sandwich the crystalline core may have an impact on that crystalline core. In isotactic polyolefins, restrictions on the relative (up/down) orientation of stems linked by a fold may result in lowered unit-cell symmetry. Also, surface stresses linked with the presence of folds determine to a large extent the non-planar shape of polymer crystals. In bulk crystallization, they may induce twisted and/or scrolled lamellae. However, this impact can be inferred only for specific polymers and/or crystal structures and/or unit-cell symmetries. (Work performed with Dr. A. Thierry and J. Ruan.)

11:39AM Z19.00003 Unexpected Observation of 2.5 Dimensional Growth of Polymer Spherulite.  
DUJIN WANG, Dr., Prof., CHANGMING WANG, YING ZHAO, JINLIANG SONG, BUXING HAN — Preparation of integrated polymer spherulite from both solution and melt has been a challenging subject. In this letter, micro-sized spherulites of ultrahigh molecular weight polyethylene (UHMWPE) have been successfully prepared from supercritical ethanol. The spherulite grows to 2.5 but not 3 dimensions with only one nucleation site on the surface. The 2.5 dimensional growth makes it possible to observe both the nucleation site and sheaf-like structure on the surface of a spherulite and to obtain one global final spherulite as a single particle. A possible mechanism for the particular morphology of spherulites is proposed based on the contributions of surface nucleation on polymer droplet, high molecular weight of UHMWPE as well as the soft confinement of supercritical fluid.

11:51AM Z19.00004 Structural evolution under uniaxial drawing of Poly(D, L-lactide) Films.  
GREGORY STOCLET, JEAN-MARC LEBREVRE, ROLAND SEGUELA, Laboratoire de Structure et Proprietes de l Etat Solide — Aliphatic polyesters are an important class of biodegradable polymers. They have drawn particular attention in the last few years as food packaging materials because they can be derived from renewable resources. Among this family, polylactide (PLA) is considered as one of the most promising “green” polymer for use as a substitute to petroleum-based polymers. In the present work, we investigate the mechanical behaviour of amorphous poly(D, L-lactide) films in relation to the structural evolution upon stretching at various draw temperatures (Td) above the glass transition temperature. Examination of the drawing behaviour shows that PLA initially behaves like a rubbery material until a true strain of the order of 1. Strain hardening occurs beyond this strain level, up to film fracture. Such strain hardening is generally ascribed to a strain induced crystallization phenomenon. In the present case, it is clearly more pronounced for Td = 90 °C than for Td = 70 °C. The corresponding structural evolutions are investigated by means of WAXS. The diffraction patterns reveal the marked influence of draw temperature. Indeed for Td = 70 °C a mesophase is induced whereas strain-induced crystallisation takes place at Td = 90 °C. Further work is in progress, in order to elucidate mesophase development and mechanical response.
12:03PM Z19.00005 Vitrification and Devitrification of Rigid Amorphous Fraction of PET during Quasi-isothermal Cooling and Heating\textsuperscript{1}, PEGGY CEBE, HUIPENG CHEN, Tufts University — Poly(ethylene terephthalate), PET, was studied by quasi-isothermal (QI) Temperature Modulated Differential Scanning Calorimetry (TM-DSC). For the first time, both the temperature dependent crystallization fraction and rigid amorphous fraction (RAF) were quantitatively analyzed during QI cooling and reheating. Specific reversing heat capacity measurements show that most RAF vitrifies step by step during QI cooling after completion of crystallization. Upon subsequent QI reheating, the RAF devitrifies also step by step and only a small RAF of 0.04 remains at 470K, while melting starts above 473K. To obtain the exact temperature of the start of melting, heat capacity measurements were made using subsequent standard DSC heating, after QI cooling. By combining this method with the QI results, the temperature dependent phase fractions were obtained during standard DSC heating. We conclude that RAF completely devitrifies before the temperature reaches the crystal melting endotherm under the conditions used in this work.

\textsuperscript{1}Research supported by the National Science Foundation, Polymers Program of the Division of Materials Research, through grant DMR-0602473 and MRI Program under DMR-0520655.

12:15PM Z19.00006 Crystallization of Model Long Chain Branched Polyethylenes with Different Branching Architectures, M. VADLAMUDI, R. G. ALAMO, FAMU-FSU College of Engineering — While the impact of long chain branching (LCB) of different architectures (stars, α − ω H type, pom-pom, combs) on rheology has been studied extensively, the effect on crystallization is less known. This work analyses the influence of LCB architecture on crystallization from quiescent melts using models based on hydrogenated polybutadienes, all with a constant 2.1 mol% of ethyl branches (LCB PEs). Crystallization rates measured by DCS, the phase structure, and morphology of the LCB PEs are studied in reference to the linear chain. At a fixed undercooling the crystallization rates of all LCB PEs are 30 to 40% lower than the rate of the linear as expected from transport limitations to the nucleation rate of the LCB systems. Smaller differences in the rate are found within the various LCB architectures. The components of the phase structure are controlled by the content of short chain branching with a negligible effect from the LCB architectures. For all LCB PEs the crystalline component is ∼30% and the interphase region ∼15% as determined by WAXD, RAMAN and DSC. A major impact of LCB is found in the supermolecular morphology. Restrictions from the LCB melt topology to propagate long organized arrays bring about a change from spherulites (linear) to poorly organized crystallites (LCB PEs). Long range dynamics (NMR T\textsubscript{2}) and lamellar structures (AFM) are presently investigated.

12:27PM Z19.00007 An anomaly in the crystallisation rate of bimodal poly(ethylene oxide) weight distributions, JESSICA L. CARVALHO, SARA L. CORMIER, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, L8S 4M1 — We present results on the crystallisation of blends of poly(ethylene oxide) (PEO) of differing molecular weight, $M_w$. Previous studies probing PEO blends have mainly focused on blends of low $M_w$, for which integral chain folding is important, with very high $M_w$. The PEO samples used in this study consist of a blend with both $M_w$'s well above the integral chain folding limit. In general, one would expect that such blends should show a monotonic decrease in spherulite growth rate, $G$, as the blend contains more high-$M_w$ component. Our results however show a clear non-monotonic $G$, with a minimum in a plot of $G$ as a function of the volume fraction. In short, blending a small amount of the low-$M_w$ into the high-$M_w$ PEO slows the growth kinetics. These results along with a possible mechanism will be discussed.

12:39PM Z19.00008 Effect of ppm Levels of Long Chain Branching on the Crystallization of Isotactic Poly(propylences) from the Melt and from Solution, RUFINA G. ALAMO, JUAN P. FERNANDEZ-BLAZQUEZ, SYED A. ABDULLAH, MADHAVI VADLAMUDI, FAMU-FSU College of Engineering — Small concentrations of long chain branching (LCB) added via copolymerization with a diene to a linear poly(propylene) chain have a dramatic effect on crystallization. LCB iPPs with diene levels between 100 and 400 ppm show greatly enhanced nucleation density, increasing with diene content. The increased nucleation observed in optical micrographs, is also evident in the crystallization half-time observed by DSC in isothermal crystallization as a function of crystallization temperature. Isotermal crystallization studies from dilute solution measured by light scattering gave the same trend with diene content and rule out any effect of gel structures affecting the nucleation rate. The linear growth rates are unchanged. The increase in nucleation rate is not linear with the increase of diene as revealed from studies of blends of LCBiPPs with the linear matrix, suggesting that length of molecules and connectivity of the LCB type, pom-pom, combs) on rheology has been studied extensively, the effect on crystallization is less known. This work analyses the influence of LCB architecture on crystallization from quiescent melts using models based on hydrogenated polybutadienes, all with a constant 2.1 mol% of ethyl branches (LCB PEs). Crystallization rates measured by DCS, the phase structure, and morphology of the LCB PEs are studied in reference to the linear chain. At a fixed undercooling the crystallization rates of all LCB PEs are 30 to 40% lower than the rate of the linear as expected from transport limitations to the nucleation rate of the LCB systems. Smaller differences in the rate are found within the various LCB architectures. The components of the phase structure are controlled by the content of short chain branching with a negligible effect from the LCB architectures. For all LCB PEs the crystalline component is ∼30% and the interphase region ∼15% as determined by WAXD, RAMAN and DSC. A major impact of LCB is found in the supermolecular morphology. Restrictions from the LCB melt topology to propagate long organized arrays bring about a change from spherulites (linear) to poorly organized crystallites (LCB PEs). Long range dynamics (NMR T\textsubscript{2}) and lamellar structures (AFM) are presently investigated.

12:51PM Z19.00009 Melting, Recrystallization and Superheating of Polymer Crystals Studied by Fast Calorimetry (1 MK/s)\textsuperscript{1}, CHRISTOPH SCHICK, ALEXANDER MINAKOV, ANDREAS WURM, EVGENY ZHURAVLEV, University of Rostock — For polymers the origin of the multiple melting peaks observed in DSC curves is still controversially discussed. This is due to the difficulty to investigate the melting of the originally formed crystals exclusively. Recrystallization is a fast process and most experimental techniques applied so far do not allow fast heating in order to prevent recrystallization totally. We developed a thin-film (chip) calorimeter allowing scanning rates as high as one million Kelvin per second. The calorimeter was used to study the melting of isothermally crystallized polymers like isotactic poly(ethyl methylenesulfone) (IPS), isotactic poly(propylene) (iPP), poly(ethylene terephthalate) (PET) and others. Our results on melting at rates as high as 1,000,000 K/s support the validity of a melting-recrystallization-melting process at low scanning rates (DSC) for all studied polymers. At isothermal conditions they form crystals, which all melt within a few dozens of K slightly above the isothermal crystallization temperature. There is no evidence for the formation of different populations of crystals with significantly different stability (melting temperatures) under isothermal conditions.

\textsuperscript{1}We gratefully acknowledge the support of DFG.

1:03PM Z19.00010 Nano-Scale Confinement Effects on Poly(ε-caprolactone) Crystallization at the Air/Water Interface, QIONGDAN XIE, BINGBING LI, TOMONORI SAITO, WEN YIN, TIMOTHY LONG, RICHARD GANDOUR, ALAN ESKER, Department of Chemistry (0212), Virginia Tech, Blacksburg, VA 24061 — Poly(ε-caprolactone) (PCL) with different mole mass were synthesized by using tri-ester primary amine as an initiator, tin(II) 2-ethylhexanoate as the catalyst, anhydrous tetrahydrofuran as a solvent at 80 °C. The three triester ε-caprolactones (PCL) with different mole mass were synthesized by using tri-ester primary amine as an initiator, tin(II) 2-ethylhexanoate as the catalyst, anhydrous tetrahydrofuran as a solvent at 80 °C. The three triester groups were further hydrolyzed to render PCL linear polymers with triacid end groups (PCL Triacid). The as-synthesized PCL triacids were attached to 9 nm magnetic nanoparticles (MNP) by ligand exchange with oleic acid in refluxing chloroform for 24 h. The crystallization behavior of PCL trihead and PCL MNPs at the air/water interface were compared with reported linear PCL crystallization. Regular crystalline morphologies observed for linear PCL are not observed for PCL-trihead and PCL-MNPs.
1:15PM Z19.00011 Microphase Separation Controlled Beta Sheet Crystallization Kinetics in Silk Fibroin Protein. XIAO HU, QIANG LU, DAVID KAPLAN, PEGGY CEBE, Tufts University — We investigate the mechanism of isothermal crystallization kinetics of beta-sheet crystals in silk multiblock fibrous proteins. The Avrami analysis kinetic theory, for studies of synthetic polymer crystal growth, is for the first time extended to investigate protein self-assembly in beta-sheet rich Bombyx mori crystallization kinetics of beta-sheet crystals in silk multiblock fibrous proteins. Observations by scanning electron microscopy support the view that the protein structures vary during the different stages of crystal growth, and show a microphase separation pattern after chymotrypsin enzyme biodegradation. We present a model to explain the crystallization of the multiblock silk fibroin protein, by analogy to synthetic block copolymers. This model could be widely applicable in other proteins with multiblock (i.e., crystallizable and non-crystallizable) domains.

1:27PM Z19.00012 Correlation between Structure and Vapor Sorption in Semi-crystalline Polymers: One Dimensional Nano-Swelling Measured using iVSANS. MAN-HO KIM, MATERIALS SCIENCE AND ENGINEERING, Northwestern University — Microemulsions and lamellar phases have been observed in previous experiments wherein block copolymers are added to blends of immiscible homopolymers. To our knowledge, all of the previous studies are restricted to homopolymers of nearly identical chain lengths with critical volume fractions in the vicinity of 0.5 (symmetric systems). The present study concerns the formation of microemulsions and lamellar phases in blends of immiscible polymers with substantial differences in chain lengths and critical volume fractions far removed from 0.5 (asymmetric systems). The characteristics of the block copolymers that enable the creation of these phases will be discussed in the presentation.

Friday, March 20, 2009 11:15AM - 2:03PM —
Session Z20 DPOLY: Polymer Blends

11:15AM Z20.00001 Microemulsions in Asymmetric Polymer Blends. ALISYN NEDOMA, Univ. of California, Berkeley, MEGAN ROBERTSON, Univ. of Minnesota, NITASH BALSARA, Univ. of California, Berkeley — Microemulsions and lamellar phases have been observed in previous experiments wherein block copolymers are added to blends of immiscible homopolymers. To our knowledge, all of the previous studies are restricted to homopolymers of nearly identical chain lengths with critical volume fractions in the vicinity of 0.5 (symmetric systems). The present study concerns the formation of microemulsions and lamellar phases in blends of immiscible polymers with substantial differences in chain lengths and critical volume fractions far removed from 0.5 (asymmetric systems). The characteristics of the block copolymers that enable the creation of these phases will be discussed in the presentation.

11:27AM Z20.00002 Nanostructured polymer blends by addition of gradient copolymer during melt mixing: Effects of copolymer sequence distribution on morphology and crystallization behavior. ROBERT SANDOVAL, JUNGKI KIM, JOHN TORKELSON, Northwestern University — Nanostructured blends of polystyrene and poly(ethylene oxide) (PEO) are produced via the addition of styrene/methyl methacrylate (S/MMA) gradient copolymer during conventional melt mixing, introducing dipole-dipole interactions between PEO and MMA repeat units. Upon addition of S/MMA gradient copolymer, stable PEO domains with diameters of ~100 nm are formed in optimized cases. This results in PEO domains homogenously crystallizing at ~20 °C, well below the crystallization temperature of bulk PEO (~50 °C). Additionally, nanostructured blends annealed at room temperature for 40 days resulted in no melting behavior upon heating, showing that the nanoconfined PEO domains remain in a rubbery state at room temperature, while bulk PEO typically remains in a crystalline state. This demonstrates that the blend properties can be easily tuned by adjusting the copolymer characteristics. This study is the first to lead to nanostructured polymer blends from non-reactive, simple melt mixing of two homopolymers and a compatibilizer.

11:39AM Z20.00003 A Morphological Study of Poly(Butylene Succinate)/Poly(Butylene Adipate) Blends with Different Blend Ratios and Crystallization Processes. JEROLD SCHULTZ, University of Delaware, HAIJUN WANG, ZHIGUA GAN, SHOUKE YAN, Chinese Academy of Sciences — Morphologies of blends of poly(butylene succinate) (PBS, m.p. 114 °C) with poly(butylene adipate) (PBA, m.p. 60 °C) varying in blend ratio and in crystallization temperature of the PBS component were studied using optical and atomic force microscopies. When PBS is crystallized at 75 °C, subsequent PBA crystallization occurs only within PBS spherulites. When PBS is crystallized at 100 °C, a portion of the PBA is rejected from the growing PBS. The morphological difference is also reflected in the time-dependence of the crystallization kinetics. The difference in behavior at these two temperatures reflects a large change in the diffusion length. Further, the location of PBA crystals within PBS spherulites depends on PBA concentration and on PBS crystallization temperature. Lower PBA concentrations lead to interlamellar segregation, while when PBA is the majority phase, interfibrillar crystallization crystallization dominates. Replace this text with your abstract body.

11:51AM Z20.00004 Phase equilibria and crystallization in mixtures of azobenzene chromophore and triacrylate. GARRETT O’MALLEY, Bucknell University, KENNETH MILAM, NAMIL KIM, THEIN KYU, University of Akron — A temperature versus composition phase diagram of azobenzene chromophore/triacrylate system was established by means of differential scanning calorimetry (DSC). The isotropic liquid (I) and crystal solid + liquid (Cr1 + I) coexistence regions bound by liquidus and solidus lines were tested with the theoretical curves obtained by self consistently solving the combined free energies of Flory-Huggins (FH) theory for isotropic mixing and phase field (PF) theory for crystal solidification pertaining to the compositional order parameter (ψ1, ψ2) and the crystal order parameter (ψ3), respectively. With the aid of phase diagram, various phase morphologies were mapped through thermal quenching into various coexistence gaps. Azobenzene in the blend produced multiple crystal structures, including gigantic single crystals. Real time images demonstrating the nucleation and growth of the crystallization process were captured using polarized optical microscopy. The spatiotemporal growth of such single crystal has been elucidated theoretically using the time-dependent Ginzburg Landau (TDGL) dynamics.

3Supported by NSF-DMR 0514942, REU DMR 0648318, and the Air Force Office of Scientific Research through the Collaborative Center for Polymer Photonics.
12:03PM Z20.00005 Miscibility Studies on Polymer Blends Modified with Phytochemicals

NEELAKANDAN CHANDRASEKARAN, THEIN KYU, The University of Akron — The miscibility studies related to an amorphous poly(amide)/poly(vinyl pyrrolidone) [PA/PVP] blend with a crystalline phytochemical called “Mangiferin” is presented. Phytochemicals are plant derived chemicals which intrinsically possess multiple salubrious properties that are associated with prevention of diseases such as cancer, diabetes, cardiovascular disease, and hypertension. Incorporation of phytochemicals into polymers has shown to have very promising applications in wound healing, drug delivery, etc. The morphology of these materials is crucial to applications like hemodialysis, which is governed by thermodynamics and kinetics of the phase separation process. Hence, miscibility studies of PA/PVP blends with and without mangiferin have been carried out using dimethyl sulfoxide as a common solvent. Differential scanning calorimetry studies revealed that the binary PA/PVP blends were completely miscible at all compositions. However, the addition of mangiferin has led to liquid-liquid phase separation and solid-liquid phase transition in a composition dependent manner. Fourier transformed infrared spectroscopy was undertaken to determine specific interaction between the polymer constituents and the role of possible hydrogen bonding among three constituents will be discussed.

12:15PM Z20.00006 Phase Separation Mechanism of Polybutadiene/Polyisoprene Blends Under Oscillatory Shear Flow

CHARLES C. HAN, Dr., Prof., RUOYU ZHANG, HE CHENG, XIA DONG, Dr., Prof. — Viscoelastic polymer blends of polybutadiene (PB)/low vinyl content polyisoprene (LPI), with a lower critical solution temperature (LCST) has been studied under oscillatory flow conditions. The phase separation mechanism has been investigated with the consideration of the nucleation mechanism, spinodal fluctuations, and also the shear induced mixing. Frequency and temperature ramping rate dependence of the apparent binodal and spinodal points will be discussed.

1 Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China.

12:27PM Z20.00007 Impact of Deuterium Substitution on the Physical Properties of Polymer Melts and Blends

RONALD WHITE, JANE LIPOSON, Dartmouth College — We examine the effects on blend properties when one of the polymeric components is deuterated. Here we use SANS-fitted model calculations to explore the underlying physical behavior, and relate our findings to subtle effects in molecular size and energetics. A special emphasis is given to the prediction and analysis of phase behavior for polymeric mixtures (e.g. liquid-liquid partial miscibility), including a comparison of phase diagrams for several related systems. We discuss effects such as pressure and molecular weight dependence and also include an analysis of calculations in which we probe the influence of key model parameters on blend miscibility. As with our earlier studies, the results featured here involve the application of a microscopically parameterized equation of state derived from an integral equation theory for lattice-based chain molecule fluids.

1 work supported by the National Science Foundation (Grant No. DMR-0502196)

12:39PM Z20.00008 Mapping Mechanical Properties and Glass Transition Temperature in Polymer Materials with sub-100 nm Resolution

MAXIM NIKIFOROV, Oak Ridge National Laboratory, STEPHEN JESSE, SANGEH GAM, RUSSELL COMPOSTO, LOUIS GERMINARIO, SERGEI KALININ, OAK RIDGE NATIONAL LABORATORY TEAM, UNIVERSITY OF PENNSYLVANIA TEAM, EASTMAN CHEMICAL CO. TEAM — Thermomechanical properties at the nanoscale are extremely important for understanding fundamental as well as technological problems. To date, Local Thermal Analysis (LTA) provides information about glass transition and melting temperature with about 1-2 µm spatial resolution. We developed LTA technique based on Scanning Probe Microscopy that allows probing not only melting and glass transition temperatures, but also elastic and loss moduli on a 100 nanometer length scale. This universal method for quantitative thermomechanical analysis was used to study the kinetics of phase separation in PMMA/SAN system. The maps of mechanical properties as function of temperature were obtained with sub-100 nm resolution. The difference of mechanical properties for two materials was determined.

1This Research at Oak Ridge National Laboratory’s Center for Nanophase Materials Sciences was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

12:51PM Z20.00009 Understanding Dynamics of Multicomponent Polymer Systems Using Homopolymer/Copolymer Blends

CALEB DYER, Department of Chemistry, Univ. of TN, DIAS LINTON, Dept. of Chemistry, Univ. of TN, MARK DAMMUN, Oak Ridge National Lab, Oak Ridge TN and Dept. of Chemistry, Univ. of TN — Blending two polymers is a cost-effective method to produce new materials with tailored properties, although the effect of the presence of one component on the dynamics of the second component is not well understood. Recent studies on miscible polymer blends show that the local environment in a polymer blend has a critical impact on the dynamics of each component in the blend. To this end we have utilized neutron reflectivity (NR), quasi-elastic neutron scattering (QENS), and rheology to study the dynamics of a polystyrene-ran-poly(methyl methacrylate) (PS-ran-PMA) copolymer in a PMMA matrix. The system consists of a miscible blend that is 90% PMMA/10% random copolymer. The copolymer composition varies from 60% to 90% MMA in the blend, effectively tuning the thermodynamic interactions in the system. We will present these results to provide insight into the role of thermodynamic interactions on the dynamics of this miscible polymer blend.

1:03PM Z20.00010 Influence of polymer chain connectivity on local composition distribution in miscible polymer blends

DMITRY BEDROV, University of Utah, WENJUAN LIU, RALPH COLBY, Pennsylvania State University — Molecular dynamics simulations using bead-necklace model have been utilized to investigate concentration distribution of local environments in model polymer blends. Distribution of effective composition around polymer segments has been investigated for different blend scenarios and bulk concentrations. Inter- and intramolecular contributions to the effective composition have been analyzed. Our analysis indicates that chains connectivity has a significant and nontrivial effect on distribution of effective composition around polymer segment. The results of this work are compared with assumptions of several theoretical models that commonly used to describe structural and dynamical correlations in miscible polymer blends.

1:15PM Z20.00011 Origins of Deviations from the RPA in Polymer Blends: Simulations and Theory

JUN KYUNG CHUNG, School of Physics and Astronomy, University of Minnesota, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — We performed continuum Monte Carlo simulations of symmetric binary polymer blends to precisely quantify deviations from RPA predictions for composition fluctuations, including critical phenomena. This comparison is made possible by an unambiguous procedure for determining the self-consistent field (SCF) χ parameter by extrapolating thermodynamic perturbation theory to the limit of infinite chain length L. Corrections to the RPA are shown to be proportional to L−1/2, and to be accurately predicted outside of the critical region by a renormalized one-loop theory. The difference between the apparent (i.e., measured) interaction parameter and the SCF value is positive (destabilizing) far from the spinodal (χN ≲ 1) as the result of an N-dependence of the depth of the correlation hole in a melt. Near the critical point, this effect is almost exactly cancelled by the stabilizing effect of long-wavelength composition fluctuations, yielding a critical value of χN quite close to the RPA prediction of (χN) ≈ 2.
1:27PM Z20.00012 Two DSC Glass Transitions in Miscible Blends of Polyisoprene / Poly(4-tert-butyl styrene), JUNSHU ZHAO, YE SUN, LIAN YU, MARK EDIGER, University of Wisconsin-Madison — Conventional and temperature modulated differential scanning calorimetry experiments have been carried out on miscible blends of polyisoprene (PI) and poly(4-tert-butyl styrene) (P4tBS) over a broad composition range. This system is characterized by an extraordinarily large component T_g difference (∼215 K) between the two homopolymers. Two distinct calorimetric T_g's were observed in blends with an intermediate composition range (25%-50% PI) by both conventional and temperature modulated DSC. Good agreement was found between the T_g values measured by the two methods. Fitting of the measured T_g's to the Lodge-McLeish model gives a φ_{eff} of 0.62~0.64 for PI in this blend and 0.02~0.05 for P4tBS. The extracted φ_{eff} for PIs comparable to reported values for PEO in blends with PMMA and is significantly larger than those reported for other PI blends with smaller component T_g differences. This observation suggests the presence of a confinement effect in PI/P4tBS blends, which results in enhanced fast component dynamics below the effective T_g of the slow component.

1:39PM Z20.00013 Segmental dynamics in polymer blends: adapting the Long-Dequeux model, GARETH ROYSTON, PAUL SOTTA, DIDIER LONG, Laboratoire Polymères et Matériaux Avancés (FRE2911) — In recent years several models have been proposed which attempt to describe the distribution of relaxation times in glass forming systems as they approach vitrification. We have adapted the Long-Dequeux model, initially proposed for van der Waals liquids, for application to polymer blends. Considering thermally induced density fluctuations, the glass transition is shown to be established by percolation of small domains of slow dynamics. Here we present a comparison of the model with experimental data including recently acquired data on miscible blends of poly(alpha-methylstyrene) and poly(cyclohexyl methacrylate). The model is shown to provide a good fit to the data over a range of conditions.

1:51PM Z20.00014 The Viscoelastic Behavior of Polymer/Oligomer Blends, WEI ZHENG, GREGORY MCKENNA, SINDEE SIMON, Texas Tech University — The dynamics in athermal blends of poly(α-methyl styrene) (PaMS) and its short chain oligomer are investigated using rheometry and differential scanning calorimetry (DSC). Master curves for the dynamic shear responses, G' and G'', are successfully constructed for both the pure materials and the blends, indicating the validity of the time-temperature superposition principle. The temperature dependence of the shift factor follows the WLF (Williams-landel-Ferry) behavior over the temperature range studied, and for the blends, the dependence is dominated by the high mobility oligomer. The discrete relaxation spectra of the materials are calculated and are found to be broader for the blends than for the pure materials. A similar domination of the dynamics by the oligomer is observed in DSC enthalpy recovery studies and in the broadened glass transition from DSC. The ability to predict the dynamic responses of the blends from the responses of the neat materials is examined, and whether this prediction needs to incorporate the self-concentration idea as described in Colmenero’s model will be discussed.

Friday, March 20, 2009 11:15AM - 1:51PM
Session Z22 GMG DMP FIAP: Focus Session: Quantum Spin Hall Effect 324

11:15AM Z22.00001 Optical Control of Topological Quantum Transport in Semiconductors, WANG YAO, The University of Hong Kong — Spin-orbit coupling enables electrical manipulations of spins, e.g. through the spin Hall effect, but it also causes spin relaxation and thus a rapid loss of information stored in spins. We propose a solution to this dilemma by exploiting light-matter interactions in the reactive regime: light is used as a control knob to switch on/off spin-orbit coupling readily without exciting real carriers. In electron-doped semiconductors, when an off-resonant optical field virtually excites interband transitions, the large spin-orbit coupling in the valence bands can be partially transferred to the photon-dressed conduction band. The adiabatic electronic ground state can thus be reactively controlled by optical pulses, exhibiting anomalous Hall conductivity. By the control of linearly polarized light, a pure spin Hall current of electrons can be driven by an in-plane DC electric field, which results in net spin accumulations at the edges of the optical excitation area. Effectively, one has created a spin battery powered by optical pulses together with DC electric field, which allows the spatial and temporal control of spin generations. The resultant electron spin accumulations can have long lifetime when spin-orbit coupling vanishes with the adiabatic switch off of the control light. Circularly polarized light breaks the time reversal symmetry and can result in spin polarized charge Hall conductance.

11:51AM Z22.00002 Spin resonance and spin-orbit coupling effects in quantum Hall edge channels1, A.V. STIER, C.J. MEINING, V.R. WHITESIDE, B.D. MCCOMBE, University at Buffalo, E.I. RASHBA, Harvard University, P. GRABS, L.W. MOLENKAMP, Universitaet Wuerzburg — We report studies of far-infrared (FIR) photo-response (E_{FIR}=3.15meV) of a 2D electron gas in an asymmetric 15nm InAs quantum well in a field/frequency regime where electron spin resonance is expected. Photo-induced changes in the longitudinal resistance were measured in a Hall-bar geometry in a tilted magnetic field (B) whose angle θ was varied. For θ ≈ 40˚ and Landau Level (LL) filling factor ν ≈ 7, we observe several sharp minima with a dominant central feature. This feature vanishes for θ < 38.4˚ and splits into two sharper lines at larger angles. The center of gravity of this pair tracks approximately the center of the ν = 7 Quantum Hall (QH) plateau. The appearance of the central feature coincides with the condition of complete filling of the ν = 7 LL at an applied B where the Zeeman spin splitting equals the energy of the FIR laser line. We attribute the sharp multiple line structure to EDSR transitions in pairs of QH edge channels whose resonance conditions are modified by Rashba effective fields. A detailed model that describes qualitatively the experimental findings will be discussed.

1Supported by DARPA ONR # N00014-00-1-0051, NSF-DMR 0203560 and NSF-ECES 0224225.

12:03PM Z22.00003 Tunneling between edge states in a quantum spin Hall system1, ANDERS STRÖM, HENRIK JOHANNESSON, Department of Physics, University of Gothenburg, Sweden — We analyze a quantum spin Hall (QSH) device with a point contact connecting two of its edges. The contact supports a net spin tunneling current that can be probed experimentally via a two-terminal resistance measurement. We find that the low-bias tunneling current and the differential conductance exhibit scaling with voltage and temperature that depend nonlinearly on the strength of the electron-electron interaction.

1Supported by the Swedish Research Council under Grant No. VR-2005-3942

12:15PM Z22.00004 Kondo effect in the helical edge liquid of the quantum spin Hall state, JOSEPH MACIEJKO, Stanford University, CHAOXING LIU, Center for Advanced Study, Tsinghua University / Stanford University, YUVAL OREG, Weizmann Institute of Science, XIAO-LIANG QI, Stanford University, CONGJUN WU, University of California, San Diego, SHOU-CHENG ZHANG, Stanford University — Following the recent observation of the quantum spin Hall (QSH) effect in HgTe/CdTe quantum wells, an important question is to understand the effect of impurities on transport in the QSH regime. Using linear response and renormalization group methods, we calculate the edge conductance of a QSH insulator in the presence of a single magnetic impurity. At high temperatures, due to Kondo scattering we find a logarithmic temperature dependence consistent with current experiments. At low temperatures, for weak Coulomb interactions in the edge liquid the conductance is restored to unitarity with unusual power-laws due to the formation of the Kondo singlet, while for strong interactions transport proceeds by weak tunneling through the impurity where only half an electron charge is transferred in each tunneling event. We propose scanning gate and shot noise experiments to search for these effects.
12:27PM Z22.00005 Corner Junction as a Probe of Helical Edge States. CHANG-YU HOU, Department of Physics, Boston University, EUN-AH KIM, Department of Physics, Cornell University, CLAUDIO CHAMÓN, Department of Physics, Princeton University — We propose and analyze inter-edge tunneling in a quantum spin Hall corner junction as a mean to probe the helical nature of the edge states. We show that electron-electron interactions in the one-dimensional helical edge states result in Luttinger parameters for spin and charge that are intertwined, and thus rather different from those for a quantum wire with spin rotation invariance. Consequently, we find that the four-terminal conductance in a corner junction has a distinctive form that could be used as evidence for the helical nature of the edge states.

12:39PM Z22.00006 A topological Dirac insulator in a quantum spin Hall phase. DAVID HSIEH, DONG QIAN, LEWIS WRAY, YUQI XIA, Department of Physics, Princeton University, YEW SAN HOR, ROBERT CAVA, Department of Chemistry, Princeton University, ZAHID HASAN, Department of Physics, Princeton University — When electrons are subject to a large external magnetic field, the conventional charge quantum Hall effect dictates that an electronic excitation gap is generated in the sample bulk, but metallic conduction is permitted at the boundary. Recent theoretical models suggest that certain bulk insulators with large spin orbit interactions may also naturally support conducting topological boundary states in the quantum limit, which opens up the possibility for studying unusual quantum Hall-like phenomena in zero external magnetic fields. Bulk Bi$_1-x$Sb$_x$ single crystals are predicted to be prime candidates for one such unusual Hall phase of matter known as the topological insulator. The hallmark of a topological insulator is the existence of metallic surface states that are higher-dimensional analogues of the edge states that characterize a quantum spin Hall insulator. Here, using incident-photon-energy-modulated angle-resolved photoemission spectroscopy, we report the direct observation of massive Dirac particles in the bulk of Bi$_0.9$Sb$_0.1$, and provide a comprehensive mapping of the Dirac insulators gapless surface electron bands. These findings taken together suggest that the observed surface state on the boundary of the bulk insulator is a realization of the topological metal.

12:51PM Z22.00007 Non-magnetic disorder effects on 3-dimensional $Z_2$ quantum spin Hall systems. RYUICHI SHINDOU, RIKEN (the Institute of Physical and Chemical Research), SHUICHI MURAKAMI, Tokyo Institute of Technology — Motivated by the recent discovery of the $Z_2$ quantum spin Hall insulator (QSHI) in the antimony doped bismuth, we have studied the non-magnetic disorder effects onto the quantum critical point (QCP) which always exists between an ordinary insulator and the $Z_2$ QSHI. Namely, intervening the topologically distinct states of matter, such QCP should be generally stable against any perturbations (i.e. disorders), as far as the time-reversal symmetry is preserved. In this talk, I will present a possible microscopic mechanism of this stability, based on simple weak-localization calculations. Specifically, at the QCP between the topological insulator and an ordinary insulator, so-called the particle degree of freedom also becomes the conserved quantity, in addition to the usual charge. As a result of this, the diffusion near the QCP consists of the two quasi-degenerate dominant contributions having the diffusion poles; one contributes to the usual charge diffusion, while the other is ascribed to the particle diffusion. In terms of these two quasi-degenerate low-energy modes, I will construct a possible microscopic picture for the stability of the QCP against non-magnetic disorders.

1:03PM Z22.00008 Magnetic impurities on the surface of a topological insulator. QIN LIU, CHAO-XING LIU, CENKE XU, XIAO-LIANG QI, SHOU-CHENG ZHANG — The surface states of a topological insulator are described by an emergent relativistic massless Dirac equation in 2+1 dimensions. In contrast to graphene, there is an odd number of Dirac points, and the electron spin is directly coupled to the momentum. We show that a magnetic impurity opens up a local gap and suppresses the local density of states. Furthermore, the Dirac electronic states mediate an RKKY interaction among the magnetic impurities which is always ferromagnetic, whenever the chemical potential lies near the Dirac point. These effects can be directly measured in STM experiments. We also study the case of quenched disorder through a renormalization group analysis.

1:15PM Z22.00009 Seeing the magnetic monopole through the mirror of topological surface states. XIAO-LIANG QI, RUN-DONG LI, Stanford University, JIADONG ZANG, Fudan University, SHOU-CHENG ZHANG, Stanford University — Existence of the magnetic monopole is compatible with the fundamental laws of nature, however, this illusive particle has yet to be detected experimentally. In this work, we show that an electric charge near the topological surface state induces an image magnetic monopole charge due to the topological magneto-electric effect. The magnetic field generated by the image magnetic monopole can be experimentally measured, and the inverse square law of the field dependence can be determined quantitatively. We propose that this effect can be used to experimentally realize a gas of quantum particles carrying fractional statistics, consisting of the bound states of the electric charge and the image magnetic monopole charge.

1:27PM Z22.00010 Theoretical study on quantum spin Hall phases in bismuth ultrathin films. SHUICHI MURAKAMI, Tokyo Institute of Technology and PRESTO, JST, MASAKI WADA, Tokyo Institute of Technology, FRANK FREIMUTH, GUSTAV BHIJMAYER, Forschungszentrum Juelich — It has been proposed that the (111) 1-bilayer bismuth is in the quantum spin Hall phase [1]. This argument is based on a simple tight-binding model for the 3D bismuth, and it is desirable to examine this result by more realistic methods. In this presentation, we investigate possibilities of the quantum spin Hall phases in two of the bismuth ultrathin films by first-principle calculations and confirmed the result in Ref.[1]. Bulk bismuth is a semimetal, while some of the bismuth ultrathin films have a gap. As proposed by first-principle calculations, among various phases seen in experiments, only two cases are gapped: (i) (111) 1-bilayer film and (ii) (012) 2-monolayer film. These two structures are almost degenerate in energy. We calculate the $Z_2$ topological numbers for the two structures, both from the bulk Bloch wavefunctions and from band structure calculations in the geometry with edges. In the calculations we use the maximally localized Wannier orbitals constructed from first-principle calculations. We found that (i) is the quantum spin Hall phase while (ii) is an ordinary insulator. Their difference can be observed in STM/STS and other possible experiments to verify our results are discussed.

1:39PM Z22.00011 Probing Surface States of the Topological Insulator Bi$_{1-x}$Sb$_x$ with Scanning Tunneling Microscopy and Spectroscopy. PEDRAM ROUSHAN, ANTHONY RICHARDELLA, COLIN PARKER, KENJIRO GOMES, ABHAY PASUPATHY, AAKASH PUSHP, YEW SAN HOR, ROBERT CAVA, ALI YAZDANI, Princeton University — There is a considerable interest in surface properties of Bi$_1-x$Sb$_x$ alloys, for which there is growing evidence that they host novel surface states [1]. We have used a cryogenic scanning tunneling microscope (STM) to probe the surface of Bi$_{1-x}$Sb$_x$ directly, and confirming the presence of surface states within the bulk band gap. Energy resolved conductance mapping of these surface states reveal strong spatial modulations, similar to those observed with the STM for noble metal surface states [2]. Fourier analysis of these maps shows that the spatial modulation of the surface states can be understood within a model for scattering between various k-states of the band structure of the surface. We will present these results in connection with the angle-resolved photoemission measurements of the contours of constant energy. [1] D. Hsieh et al., Nature 452, 970 (2008) [2] M. F. Crommie et al., Nature 363, 524 (1993)
11:15AM Z24.00001 Effect of Ti Dopant on Surface Diffusion of Isolated Alane Species: A Comparison between Al (111) and Al (100) surfaces1, ALTAF KARIM, JAMES MUCKERMAN, Brookhaven National Lab — Our density functional theory-based kinetic Monte Carlo simulations show that an embedded Ti atom creates a well in the potential energy surfaces of Al(111) and Al(100) as probed by hydrogen and other isolated alanine species. Hydrogen adatoms become trapped around Ti atoms on an Al(111) surface, whereas Al adatoms do not exhibit any significant effect of the potential energy well created by the Ti atoms. In contrast to the case of Al(111), Al adatoms on an Al(100) surface also become trapped around the Ti atoms for a longer period of time compared to the hydrogen adatoms on this surface. Therefore, Ti sites on Al(100) become poisoned by the presence of Al adatoms around them for long periods of time, thereby blocking further dissociative adsorption of hydrogen. The overall diffusion of Al adatoms on an Al(100) surface is significantly lower compared to the Al(111) surface. This fact suggests that the Ti-doped Al(111) surface is perhaps more conducive to the production of alanine species than the Ti-doped Al(100) surface despite its higher activation barrier for the dissociation of molecular hydrogen.

1DOE Contract No. DE-AC02-98CH10886 and a DOE BES Hydrogen Fuel Initiative award (BO-130) using the NERSC computational resources

11:27AM Z24.00002 Hydrogen adsorption on Al (100) facilitated by surface alloying with Sc. FENG ZHANG, YAN WANG, M. Y. CHOU — We report first-principles investigations of hydrogen adsorption on the Al (100) surface modified by alloying with Sc, as the first step to understand the catalytic role of scandium in the hydrogenation process in Sc-doped NaAlH4. Sc prefers to stay at subsurface sites with or without adsorbed hydrogen. The adsorption energy on the Sc-modified surface is 0.5 eV/H2 lower than that on the pure Al surface, while the dissociation barrier of H2 is similar for the two systems. The structure with two H atoms adsorbed on two nearest-neighbor bridge sites is at least 0.3 eV more stable than other structures, but no additional activation energy is required for H to diffuse among these structures. Electronic structures are also examined to explain these alloying-induced effects.

11:39AM Z24.00003 Hydrogen-related defects and the role of metal additives in complex hydrides1, KHANG HOANG, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — Complex hydrides such as NaAlH4 and LiBH4 have attractive properties as hydrogen storage materials. The mechanism of the enhancement in (de)hydrogenation rates caused by these metals is, however, not well understood. We have carried out first-principles studies based on density functional theory of hydrogen vacancies and interstitials, which play an important role in the (de)hydrogenation processes. We find that these defects are always charged, their formation energy therefore depends on the Fermi level. The metallic impurities can also exist in different charged states and, therefore, modify the Fermi level, thus changing the defect concentrations. Our first-principles results shed light on the role of transition-metal impurities in hydrides and lead to the design of storage materials with improved characteristics.

1Work supported by General Motors.

11:51AM Z24.00004 First-principles and Tight-binding Calculations in the Pd-H System, A. SHABADEV, D.A. PAPCONSTANTOPOULOS, Department of Computational and Data Sciences, George Mason University, Fairfax, VA 22030, USA — Using the linearized augmented plane wave(LAPW) method we have generated a large database of electronic structure results that include fcc, bcc, NaCl, CsCl, CuAu. Fluorite crystal structures as well as supercell configurations with various hydrogen occupations for the Pd-H system. The formation energies and energy bands from this database were used to construct a tight-binding model that reproduces well the above LAPW results and, in addition, is transferable to other crystal lattices including random occupation of crystal sites as well as treating vacancies. We calculate the phonon frequencies, elastic constants, the density of states, coefficient of thermal expansion, mean-squared displacement and the energy of vacancies formation in Pd. The objective of this work is to be able to perform electronic structure calculations for systems containing up to a few thousand atoms where first-principles calculations are computationally intractable. This approach is used in both static and dynamic calculations and enables us to vary the amount of hydrogen entering into the Pd matrix.

12:03PM Z24.00005 Nitrogen and Hydrogen on a Palladium-covered proton conductor: a first principle study of Ammonia catalysis, LORENZO PAULATTO, STEFANO DE GIRONCOLI, SISSA, I-34014 Trieste and DEMOCRITOS I-34014 Trieste — Being liquid at ambient conditions Ammonia would be an ideal Hydrogen vector. However, the industrial Haber process for Ammonia synthesis involves high pressures (≥ 100 bar) and temperatures (450 – 500 °C), making the process very expensive. Recently, ambient pressure Ammonia production, in the 570 – 750 °C temperature range, has been reported at the Palladium cathode of a proton conducting cell-reactor [1]. The rate limiting step in the Haber process is N2 dissociation, while the observed limiting factor in Ref. [1] appears to be the proton transfer through the conductor and it has been proposed that Nitrogen hydrogenation may in this case precede dissociation. We use first-principles techniques to study Nitrogen, Hydrogen and Ammonia interaction with flat and stepped Pd surfaces, in presence of external electric fields. Our aim is to study the effect of electrochemically provided protons on the catalysis of the reaction. [1] G. Marnellos and M. Stoukides, Science 282, 98 (1998); G. Marnellos, S. Zisekas, and M. Stoukides, J. of Catalysis 193, 8087 (2000)

12:15PM Z24.00006 Synthesis and Characterization of Au and Pd Decorated ZnO Powders1, PAIGE LANDRY, University of Tennessee, HANGNING CHEN, Lanzhou University, University of Tennessee, ANDI BARBOUR, MICHAEL FELTY, University of Tennessee. — We report our synthesis and characterization of ZnO nanopowders decorated with Pd and Au clusters. Ultrapure ZnO powders are readily produced. Pd and Au nanoclusters are deposited from solution and reduced using hydrogen gas. Characterization of these materials using high resolution adsorption isothersms and inelastic neutron scattering have been performed. Particular attention has been paid to the adsorption of hydrogen and deuterium on these pure and decorated materials. Preliminary results indicate that hydrogen preferentially adsorbs on Pd and Au nanoclusters. Ultrapure ZnO powders are readily produced. Pd and Au nanoclusters are deposited from solution and reduced using hydrogen gas.

1Supported by U.S. DOE, Materials Science Division under contract No. DE-AC05-00OR22725 with Oak Ridge National Laboratory, and the NSF under grant DMR-0412231


11:15AM Z25.00001 Chiral structure and mixed parity anomalies in graphene-related systems, AKIHIRO TANAKA, Natl. Inst. for Materials Sci. — We reanalyze the chiral symmetry structure of graphene and its variants (boron-nitride sheets, bond alternated graphene, etc) using a representation of Dirac fermions previously employed by the author in a search for topological effects in the pi- flux state of a square lattice electron system (PRL 95 036402 (2005)). We find that the electromagnetic responses of nontopological insulators to curvature-induced gauge fields mimics in an interesting way the responses of topological insulators of the Haldane/Kane-Mele category to conventional (Maxwellian) gauge fields.
Our energetics calculations show that the OH group tends to aggregate to the neighboring carbon sites of an epoxy group, resulting in the formation of several effects of the oxidation functional groups (epoxy and hydroxyl) on the structural, energetics, and electronic properties of graphene by first-principles calculations.

JIA-AN YAN, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — Opening a band gap in monolayer graphene is of and thus generate a big perturbation on graphene Dirac point energy level. Here we show that physical adsorption of suitable aromatic molecules onto graphene can generate a moderate band gap of approximately 0.125 eV, with an gap opening near the Fermi level. The oxidation concentration dependence of the energy gap is investigated.

WANLIN GUO, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — We explore the response of epitaxial bilayer graphene on SiC and Ru to electric field and mechanical tuning using first-principles calculations. Our calculations reveal that, in contrast to prevailing view, the buffer layer plays an active role in the distribution of charge transfer within the epitaxial graphene layers and with the substrate. The charge distribution and electronic structure are also sensitive to the type of substrate. These results provide new insights for fundamental understanding and practical application of these fascinating materials.

ANTONIO J. R. DA SILVA, Physics Institute, University of São Paulo, São Paulo, Brazil — Single layer graphene has been recently isolated and can pave the way to a number of nanoscale technologies. One interesting possibility is to use the spin of the electron - instead of its charge - as information carrier in carbon-based systems where the spin coherence length can reach hundreds of nanometers. Up until now, spintronics devices have been assembled using magnetic electrodes as a source of spin polarized electrons. In this work we use a combination of density functional theory and nonequilibrium Green’s functions techniques to study the electronic transport properties of graphene nanoribbons (GNRB) up to 500 nm long containing substitutional Boron atoms. We demonstrate that in realistic systems where the B atoms are randomly distributed along the GNRB, the polarization of the current can reach up to 100% and is independent of impurity concentration. These effects can be explained in terms of different scattering probabilities for majority and minority spins from a single B atom. This consequently leads to different Anderson localization lengths for each spin population.

MICHELE LAZZERI, IMPMC, Paris, France, CLAUDIO ATTACALITE, ETSF, Universidad del Pais Vasco, Spain, LUDGER WIRTZ, IEMN, ISEN, Villeneuve d’Asq, France, ANGEL RUBIO, ETSF, Universidad del Pais Vasco, Spain, FRANCESCO MAURI, IMPMC, Paris, France — GW is nowadays the most accurate ab-initio method to determine electronic bands. So far GW has never been used to determine neither the electron-phonon coupling (EPC) nor phonon dispersions. We show that GW approach [1] can be used to compute the EPC and the phonon dispersion. In particular, in graphene and graphite, standard DFT (LDA and GGA) underestimates, by a factor of 2, the slope of the highest optical branch at the zone boundary (K) and the square of its EPC by almost 80%. On the contrary, GW reproduces the experimental phonon dispersion near K, the value of the EPC, and the electronic band dispersion, in agreement with phonon dispersions from inelastic x-ray scattering and Raman spectroscopy. Comparing these results with other computational methods, the B3LYP hybrid functional gives phonons close to GW but overestimates the EPC at K by about 30%. Within Hartree-Fock, the graphene structure displays an instability under a distortion following the A'1 phonon at K. [1] M. Lazzzieri et al., Phys. Rev. B 78, 081406(R) (2008).

11:27PM Z25.00002 Many-electron Effects on the Electronic Structure and Optical Spectrum of Few-layer Graphene, LI YANG, JACK DESLIPPE, CHEOL-HWAN PARK, MARVIN COHEN, STEVEN LOUIE, The department of Physics, University of California at Berkeley and Materials Sciences Division, Lawrence Berkeley National Laboratory — We present a first-principles calculation of the optical properties of single- and few-layer graphene with many-electron effects included, employing the GW-Bethe Salpeter equation (GW- BSE) approach. We have found enhanced excitonic effects that result in significant changes in the optical absorption of few- layer graphene as compared to the independent-particle picture. Our calculated absorption spectrum is in good agreement with recent experiments. This study is of importance for understanding excitonic effects in two-dimensional semimetal systems and expected to be useful for possible optoelectronics applications of graphene.

11:39AM Z25.00003 Geometrical constraint on alkali and halogen adsorption on graphene, CHENGING CHIA, Department of Physics, Penn State University — A seamless sp2 graphene sheet prevents the penetration of atoms through the sheet, yet allows the penetration of electrons. Thus, a suspended single sheet graphene forms a geometrical constrained background by separating the surrounding vacuum into upper half and lower half spaces. Alkali and halogen atoms, each constrained to one of the spaces, are forced to interact electrostatically via charge transfer through the sheet. A new type of chemical interaction is formed under this constraint, which we call topologically frustration bonding. We have calculated the interaction of a K atom on the upper surface with a halogen atom on the lower surface of a pure-carbon graphene sheet using density functional theory. The system becomes ferroelectric under this new geometrical constraint.

11:51AM Z25.00004 Pivotal role of buffer layer in tuning electronic properties of epitaxial graphene, YUFENG GUO, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA, WANLIN GUO, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA — We explore the response of epitaxial bilayer graphene on SiC and Ru to electric field and mechanical tuning using first-principles calculations. Our calculations reveal that, in contrast to prevailing view, the buffer layer plays an active role in the distribution of charge transfer within the epitaxial graphene layers and with the substrate. The charge distribution and electronic structure are also sensitive to the type of substrate. These results provide new insights for fundamental understanding and practical application of these fascinating materials.

12:03PM Z25.00005 Graphene on Silicon Dioxide: Band gap modulation via substrate surface chemistry, PHILIP SHEMELELLA, SAROJ K. NAYAK, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY — We have studied the electronic structure of graphene deposited on a SiO2 surface using density functional methods. The band structure of the graphene monolayer strongly depends on surface characteristics of the underlying SiO2 surface: for an oxygen-terminated surface, the monolayer exhibits a finite energy band gap while the band gap is closed when the oxygen atoms on the substrate are passivated with hydrogen atoms. We find that at least a graphene bilayer is required for a near zero energy gap when deposited on a substrate without H-passivation. Our results are discussed in the light of recent experiments.

12:15PM Z25.00006 Current polarization in B-doped graphene nanoribbons: ab initio simulations, ALEXANDRE ROCHA, Centro de Ciências Naturais e Humanas, UFABC, Santo André, Brazil, THIAGO MARTINS, ADALBERTO FAZZIO, ANTONIO J. R. DA SILVA, Physics Institute, University of São Paulo, São Paulo, Brazil — Single layer graphene has been recently isolated and can pave the way to a number of nanoscale technologies. One interesting possibility is to use the spin of the electron - instead of its charge - as information carrier in carbon-based systems where the spin coherence length can reach hundreds of nanometers. Up until now, spintronics devices have been assembled using magnetic electrodes as a source of spin polarized electrons. In this work we use a combination of density functional theory and nonequilibrium Green’s functions techniques to study the electronic transport properties of graphene nanoribbons (GNRB) up to 500 nm long containing substitutional Boron atoms. We demonstrate that in realistic systems where the B atoms are randomly distributed along the GNRB, the polarization of the current can reach up to 100% and is independent of impurity concentration. These effects can be explained in terms of different scattering probabilities for majority and minority spins from a single B atom. This consequently leads to different Anderson localization lengths for each spin population.

12:27PM Z25.00007 Impact of the electron-electron correlation on phonon dispersion: Failure of LDA and GGA DFT functionals in graphene and graphite, MICHELE LAZZERI, IMPMC, Paris, France, CLAUDIO ATTACALITE, ETSF, Universidad del Pais Vasco, Spain, LUDGER WIRTZ, IEMN, ISEN, Villeneuve d’Asq, France, ANGEL RUBIO, ETSF, Universidad del Pais Vasco, Spain, FRANCESCO MAURI, IMPMC, Paris, France — GW is nowadays the most accurate ab-initio method to determine electronic bands. So far GW has never been used to determine neither the electron-phonon coupling (EPC) nor phonon dispersions. We show that GW approach [1] can be used to compute the EPC and the phonon dispersion. In particular, in graphene and graphite, standard DFT (LDA and GGA) underestimates, by a factor of 2, the slope of the highest optical branch at the zone boundary (K) and the square of its EPC by almost 80%. On the contrary, GW reproduces the experimental phonon dispersion near K, the value of the EPC, and the electronic band dispersion, in agreement with phonon dispersions from inelastic x-ray scattering and Raman spectroscopy. Comparing these results with other computational methods, the B3LYP hybrid functional gives phonons close to GW but overestimates the EPC at K by about 30%. Within Hartree-Fock, the graphene structure displays an instability under a distortion following the A1 phonon at K. [1] M. Lazzzieri et al., Phys. Rev. B 78, 081406(R) (2008).

12:39PM Z25.00008 First-Principles Studies of Oxidation Functional Groups on Graphene, JIA-AN YAN, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — Opening a band gap in monolayer graphene is of special interest for the graphene-based electronic applications. Inspired by the potential applications of graphene oxide, we have systematically investigated the effects of the oxidation functional groups (epoxy and hydroxy) on the structural, energetic, and electronic properties of graphene by first-principles calculations. Our energetic calculations show that the OH group tends to aggregate to the neighboring carbon sites of an epoxy group, resulting in the formation of several possible building units. We find that the epoxy group strongly hybridizes with the extended π (nπ) bands, giving rise to a shift of the Dirac point in the momentum space and a decrease in the Fermi velocity. In contrast, the adsorption of a single hydroxyl group leads to the formation of a localized state and a gap opening near the Fermi level. The oxidation concentration dependence of the energy gap is investigated.

12:51PM Z25.00009 Physical adsorption induced band gap opening in graphene, YOUJIAN TANG, Penn State, VINCENT CRESPI, VINCENT CRESPI GROUP TEAM — Gapping graphene is crucial for enabling its use in next-generation electronic devices. Here we show that physical adsorption of suitable aromatic molecules onto graphene can generate a moderate band gap of approximately 0.125 eV, with an adsorption energy 0.67 eV. The reason for such a band gap is that the Lowest unoccupied molecular orbit of adsorbate is right across the Fermi level of graphene and thus generates a big perturbation on graphene Dirac point energy level.
1:03PM Z25.00010 First-Principles Studies of Covalent Functionalization of Graphene by Carboxyl Groups1, NABIL AL-AQTASH, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, New Mexico — We study the mechanism of covalent functionalization of graphene by the carboxyl (COOH) group in the framework of density functional theory combined with the generalized gradient approximation. The structures and binding energies of the COOH group attached to the surface of graphene are examined in cases of graphene containing no defects, containing a Stone-Wales defect, and containing a vacancy. Our calculations confirm that the binding of the COOH group with graphene is significantly stronger in the presence of surface defects. We also observe substantial changes in the structure of defective graphene after the attachment of the COOH group. These results suggest that surface defects play an important role in the carboxylation of graphene.  

1Supported by DOE DE-FG36-08GO80008 and ACS PRF-48556-AC10.

1:15PM Z25.00011 First-principles calculations of electronic transport through graphene with realistic metallic leads, SALVADOR BARRAZA-LOPEZ, M. Y. CHOU, School of Physics, Georgia Institute of Technology — We present transmission characteristics for electrons through graphene with realistic metallic contacts. The methodology relies on an in-house version of the electronic transport SMEAGOL code [1], in which the memory required to allocate for the matrices of contact leads and the graphene sheet in the Green’s function solver is distributed into more than one processor, for a given electron energy. We are able to accommodate for commensurate graphene-metal supercells which have the correct atomic structure (namely, stress caused by contracting/ extending the metal contacts to match the periodicity of graphene is avoided). In addition, and despite of the large size of the leads, the electronic properties and transport are computed at the density-functional theory level [2] within a double-zeta plus polarization basis[3], ensuring the accuracy of the atomic forces in the system, as well as on the final transmission characteristics. [1] A. R. Rocha et al, PRB. 73, 085414 (2006); [2] J. M. Soler et al, J. Phys.: Condens. Matter 14, 2745-2779 (2002); [3] J. Junquera et al, PRB 64, 235111 (2001).

1:27PM Z25.00012 Exfoliation of graphene flake from SiC substrate using hydrogen injection; a first-principle study, BORA LEE, SEUNGWU HAN, Ewha Womans University, YONG-SUNG KIM, Korea Research Institute of Standards and Science — Recently there is an immense interest in studying graphene for investigating its unique electronic properties as well as practical applications to nanoscale devices. Up to now there are two methods to obtain graphene layers. The first one is a mechanical method in which the single graphene sheet is split off the bulk graphite crystals using adhesives. The other method is graphitization of SiC surfaces by annealing at elevated temperatures. Even though the latter approach can provide a graphene layer in a more controlled way, the exfoliation of the graphene layer still poses a big challenge. In this presentation, based on the first-principles results, we propose a novel exfoliation method using hydrogen. As a model system, the 6H-SiC(0001) 4×4 cell is used, which corresponds to the 3×3 graphene cell. We calculate the binding energy of single hydrogen atom in various places; above and below graphene surface and inside the first SiC layer. The binding energies of hydrogen are calculated for different coverages. It is found that at high coverages, the hydrogen atoms prefer to bind below the graphene surface, cutting the graphene-SiC bonds. This means that the graphene can be exfoliated in the hydrogen-rich environment. The detailed analysis including the electronic structures will be presented.

1:39PM Z25.00013 Electronic Properties of Graphene Oxide1, GEUNSIK LEE, KEEONGJAE CHO, Department of Physics, UT Dallas, TX 75080 — Graphene has shown promising electronic properties as future device applications beyond the current CMOS (complimentary metal-oxide-semiconductor) technology based on silicon microelectronics. As a critical insulating component in all-carbon nanoelectronic devices, graphene oxides (GOs) are shown to have insulating behavior, but their electronic and atomic structures are poorly understood. We investigated electrical property of GO using density functional theory (DFT) and non-equilibrium Green’s function (NEGF) method with tight binding (TB) scheme. We model the basal plane oxidation with top (OH) and bridge (epoxide) chemisorptions. By varying the chemisorption ratio of the hydroxyls and epoxides as well as their coverage, the conductance of GO is calculated and quantitatively compared with experimental reports. We have investigated the electronic structure of graphene and GO multilayers for pseudospin device application.

1This research is supported by the NRI SWAN funding.

1:51PM Z25.00014 Lattice Monte Carlo studies of quantum critical phenomena in graphene, TIMO LAHDE, University of Washington, JOAQUIN DRUT, The Ohio State University — The Lattice Monte Carlo approach is well suited to the study of strongly interacting fermionic systems, such as the quasi-relativistic charge carriers in graphene, as it is non-perturbative and takes full account of quantum fluctuations. Recent simulational results on the semimetal-insulator critical point in graphene are presented, with emphasis on the question whether the transition to an insulating phase is of second order or of first order. This critical point is likely to be relevant for the physics of suspended graphene, as its location determined in arXiv:0807.0834 (see abstract by J. E. Drut) suggests that suspended graphene should be an insulator rather than a semimetal. An observable of particular interest is the DC conductivity of graphene, as most analytical studies underestimate this by a factor ~3. It has been pointed out that a complete description of the DC conductivity of graphene should account for non-perturbative effects due to the long-range Coulomb interaction between the fermionic quasiparticles. A possible method for determining the DC conductivity of graphene using the Lattice Monte Carlo technique is presented.

Friday, March 20, 2009 11:15AM - 2:15PM – Session Z26 DCMP: Composite and Porous Media 328

11:15AM Z26.00001 Flexibility of zeolite frameworks, VITALIY KAPKO, MICHAEL TREACY, MICHAEL THORPE, Department of Physics Arizona State University — Zeolites are an important class of industrial catalysts because of their large internal surfaces and molecular-sieving properties. Recent geometric simulations [1] show that almost all of the known zeolites can exist without distortion of their tetrahedra within some range of densities, which we call the flexibility window. Within this window, the framework accommodates density changes by rotations about the shared Si-O-Si bonds. We are able to accommodate for commensurate graphene-metal supercells which have the correct atomic structure (namely, stress caused by contracting/ extending the metal contacts to match the periodicity of graphene is avoided). In addition, and despite of the large size of the leads, the electronic properties and transport are computed at the density-functional theory level [2] within a double-zeta plus polarization basis[3], ensuring the accuracy of the atomic forces in the system, as well as on the final transmission characteristics. [1] A. R. Rocha et al, PRB. 73, 085414 (2006); [2] J. M. Soler et al, J. Phys.: Condens. Matter 14, 2745-2779 (2002); [3] J. Junquera et al, PRB 64, 235111 (2001).

11:27AM Z26.00002 Electronic and ionic conduction in oxo-vanadium arsenates, VICTORIA SOGHOMONIAN, Vincenzo Tech, Department of Physics — Oxides conducting microporous zeolite-like or zeolite frameworks are widely studied as electronic materials, but may offer new avenues in catalysis and in electrical energy storage applications. Zeolites and zeotypes are characterized by the presence of nano channels and cavities delineated by their crystalline framework, and occur naturally or can be synthesized by inorganic methods. The material under discussion here, an oxo-vanadium arsenate system, combines the properties of the well known but electrically insulating microporous zeolites, with an electronically active framework. We present the structure and the experimentally measured electronic and ionic conductivities of the materials system, the temperature dependences of the conductivities, and discuss possible electronic and ionic conduction mechanisms at play in empty frameworks and ion-exchanged frameworks. We also discuss how microporous electrically conducting frameworks can find use in electrical energy storage, and compare the zeolite frameworks in such applications to other materials systems such as mesoporous carbon.
11:39AM Z26.00003 Synthesis of hybrid zeolite materials with TiO2 nanocrystals using solid-solid method1, CORINA ORHA, CARMEN LAZAU, CORNELIA RATIU, PAULA SFIRLOAGA, PAULINA VLAZAN, ALEXANDRA IOITESCU, National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania — Zeolite seems to be a promising support for TiO2 photocatalyst because of its regular pores and good adsorption ability. TiO2 supported on zeolite integrates the photocatalytic activity of TiO2 with the adsorption properties of zeolites. The aim of this paper was the syntheses and characterizations of functionalized zeolite materials with undoped, Fe-doped and N-doped TiO2 nanocrystals. The zeolite hybrid materials impregnation with titanium dioxide was achieved through solid-solid method. TiO2 doped with metallic (Fe) and non-metallic (N) ions was obtained directly from precursors by sol-gel and hydrothermal methods. The hybrid materials were characterized by XRD, SEM with EDAX, IR and AFM.

1National Project ZEONANO-SPP, 56/2007

11:51AM Z26.00004 Carbon dioxide and methane transport in DDR zeolite: insights from molecular simulations into carbon dioxide separations in small pore zeolites, SANG EUN JEE, DAVID SHOLL, Georgia Institute of Technology, EXXON MOBIL CORPORATION COLLABORATION — Zeolites are good candidates as a membranes for chemical separations because of their excellent chemical and thermal stability. Cage type zeolites are promising materials for gas separation since their narrow windows are expected to control molecular transport. DDR is one of the strongest candidates for light gas separations because of its narrow 8MR window. In our study, we examined the separation selectivity of DDR for CO2/CH4 separation using atomistic simulation methods. We introduced new force fields which can reproduce experimental single component adsorption and diffusion data for this material for the first time. Previously interatomic potentials that have been applied to DDR overestimate experimental diffusivities at least one order of magnitude. We characterized single-component and binary adsorption using Grand Canonical Monte Carlo, and single-component diffusion using a combination of Molecular Dynamics and Transition State Theory. The most important observation from our calculation is that CO2/CH4 diffusion in DDR is very different from the usual situation in nanoporous materials, where the presence of a slowly diffusing species retards transport rates of a more rapidly diffusing species. In DDR, we show that CO2 diffusion rates are only weakly affected by the presence of CH4, despite the very slow diffusion of the latter species. The physical origins of this unusual behavior are explained by analyzing the adsorption sites and diffusion mechanism for each species.

12:03PM Z26.00005 Effects of inhomogeneous partial absorption and the orientation of the boundary on the population evolution of molecules diffusing in general porouos media, SEUNGHO RYU, DAVID L. JOHNSON, Schlumberger Doll Research — We consider the diffusion-relaxation dynamics in porous media with partially absorbing boundary conditions. Spectral analysis of Helmholtz equation for the uniform boundary condition has been widely used as a probe of geometry of the medium. The NMR relaxation of the fluid magnetization, for example, is used for a variety of media such as rocks, cement, bones, and cheese. While direct relationship between their geometry and the spectrum forms the basis for such applications, little attention has been paid to the spatial variation of the boundary condition. We report on the way the geometry and such inhomogeneity become intertwined and affect the spectrum. It is often impossible to gauge how severe such interference is in the biological or geophysical experiments. We develop a perturbative theory and numerical techniques and test for cases for which exact solution is obtained.

12:15PM Z26.00006 Decomposing First Passage Random Walks, LAWRENCE SCHWARTZ, DAVID JOHNSON, Schlumberger, SIDNEY REDNER, Boston University — We develop a simulation method to model the time dependence of diffusion in composite materials with a wide range of pore sizes. Here, first passage techniques are useful because they allow a walker to move efficiently through the large open regions of the pore space. However, because one does not keep track of each intermediate position, these techniques are not well suited to calculating the effective diffusion coefficient, D(t). To address this problem we show that first passage propagation can be decomposed in terms of a sequence of intermediate probability distributions. For example, given a first passage walk from the origin to the surface of a sphere of radius R in a time t, we can evaluate the probability distributions for the particle's location at any earlier time t'. We will illustrate the behavior of these intermediate distributions with a series of examples in one and three dimensions.


12:27PM Z26.00007 Thermally Stable Mesoporous Silica Spheres synthesized under Mild Conditions1, CHRISTOPHER ZIEGLER, EUNYOUNG YOU, JAMES WATKINS, University of Massachusetts Amherst — Thermally stable, mesoporous silica spheres were synthesized using a one-pot technique under mild conditions. As-calced silica spheres were shown to be highly porous with surface areas greater than 1000 m2/g and pore volumes on the order of 1 cc/g. Pore walls were found to be highly resistant to collapse as a consequence of thermal treatment at temperatures exceeding 750 °C or hydrothermal treatment in boiling water at temperatures exceeding 100 °C for over 100 hours. 29Si-1H cross polarization NMR data indicate that the silica is highly condensed at the surface providing rationale for the exceptional pore wall stability observed. The mesoporous silica spheres were synthesized from tetraethyl orthosilicate (TEOS) at room temperature and near-neutral pH using cysteamine and cetyltrimethylammonium bromide (CTAB) in a mixed water and ethanol system. Sphere diameters ranging from 30 nm to 560 nm were observed. The preparation method and characterization of functionalized zeolite materials with

1AFOSR, MRSEC, NSEC

12:39PM Z26.00008 Ordered and disordered pores in porous anodic alumina: Partial equilibrium results from hexagonal lattice1, ARIEF BUDIMAN, DANIEL LO, University of Calgary — Cluster variation method is employed to find equilibrium states of pore arrangement in porous anodic alumina. Our work is motivated by a need to predict the extent of pore ordering in the anodic alumina. The pores are assumed to occupy a hexagonal two-dimensional lattice and interact with each other through their elastic deformations. Alumina-electrolyte interface energy and metal-oxide interface stress are included in the analysis. Equilibrium ordered and disordered states are obtained. Spatial pore arrangements of these states will be presented. Incorporation of ionic transports in the electrolyte and aluminum-to-alumina reactions to the model will be discussed.

1We acknowledge the financial support of NSERC.
12:51PM Z26.00009 Nanoporous Substrate with Mixed Nanoclusters for Surface Enhanced Raman Scattering. SEHOOON CHANG, Georgia Institute of Technology, HYUNHYUB KO, UC Berkeley, SRIKANTH SINGAMANENI, RAY GUNAWIDJAJA, VLADIMIR TSUKRUK, Georgia Institute of Technology — Rapid detection of plastic and liquid explosives is an urgent need due to various societal and technological reasons. We employed a novel design of surface enhanced Raman scattering (SERS)-active substrate based on porous aluminia membranes decorated with mixed nanoclusters of gold nanorods and nanoparticles. We demonstrated trace level detection of several important explosives such as dinitrotoluene (DNT), trinitrotoluene (TNT), and hexamethylenetriperoxidediamine (HMTD) by fast, sensitive, reliable Raman spectroscopic method. We achieved near molecular-level detection (about 15 ~ 30 molecules) of DNT and TNT utilizing the SERS substrate. However, trace level detection is challenging due to the lack of common optical signatures (fluorescence, absorption in UV-vis range) or chemical functionality of peroxide-based explosives such as HMTD. To overcome this, we employed photochemical decomposition approach and analyzed chemical fragments using SERS. We suggest that tailored polymer coating, mixed nanoclusters, and laser-induced photocatalytic decomposition are all critical for achieving this unprecedented sensitivity level.

1:03PM Z26.00010 Sorption Isotherms in Networked Nanoporous Media: Do the Parts Equal the Whole?1. CASEY E. CHIANG, FELIX CASANOVA, ANNE M. RUMINSKI, MICHAEL J. SAILOR, IVAN K. SCHULLER, University of California-San Diego — Sorption isotherms are a very important tool in the characterization of nanoporous materials. However, there is still controversy as to how capillary condensation and evaporation transitions along the isotherm correlate with the pore morphology (shape) and topology (within a network). We combined narrow (<10 nm) and wide (>30 nm) pores in nanoporous silicon to tailor the simplest networks: narrow above wide (ink-bottle) and vice versa (funnel). In addition, we compared these against their single-layered constituents. From sorption isotherms measured by optical interferometry, we observe that capillary condensation occurs identically in all pores with direct access to the gas reservoir and delayed (pore-blocking) when access is blocked, while capillary evaporation occurs identically in all pores with direct access to the gas reservoir and is delayed (pore-blocking) until direct access is allowed otherwise. These experimental results allow us to understand the global capillary behavior in nanoporous silicon.

1Work supported by AFOSR and California Space Grant Consortium.

1:15PM Z26.00011 Mechanical stability of Metal Organic Framework-5. WEI LIU, JU LI, University of Pennsylvania — Metal organic frameworks (MOFs) are crystalline structures of metal ions bridged by organic linkers. They have been proved to be highly useful in gas storage, separation, purification and catalysis. Mechanical stability is very important for their applications in industry. We studied the stress-strain relations of MOF-5 (the prototypical MOF) under different temperatures via Molecular Dynamics method (MD). It has been found that under normal stress MOF-5 is relatively strong; while under shear stress it is easy to collapse. Furthermore, under both normal and shear stress condition, its stability becomes weaker as temperature increases.

1:27PM Z26.00012 Smart nanoporous preconcentrator of explosives based on MOF51, KHORGOLKHHUU ODBADRAKH2, JAMES LEWIS, WVU — We present investigations of interactions of explosive molecules RDX and TATP with metal organic framework MOF-5, using DFTY based ab-initio simulation method FIREBALL. Energetics studies in bulk shows that only one of the binding sites of RDX in MOF-5 suggested by quantum chemistry calculations confirm. The absorption site is on a linker of the framework through 2-(OH) bond. However, surface interactions are stronger, with significantly higher binding barriers. We confirmed two adsorption sites on the surface: one with the linker and the other on a connector of the framework through 3-(OH) bonds. The stronger interactions on the surface suggest importance of size, and surfaces of MOF nanoparticles in preconcentrating the explosive molecules in the framework. Ab-initio Molecular Dynamics simulations show that the absorption of the RDX in MOF-5 is highly sensitive to temperatures, suggesting high diffusion rates for the explosive molecules at room temperature.

1NSF EXP-LA
2corresponding author

1:39PM Z26.00013 Optical birefringence in Compressed Aerogels1, P. BHUPATHI, J. HWANG, R. M. MARTIN, L. JAWORSKI, D. B. TANNER, Y. LEE, Department of Physics, University of Florida, Gainesville, FL 32611, J. BLANKSTEIN, Alexander W. Dreyfoos School of the Arts, West Palm Beach, FL 33401, N. MULDERS, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 — We performed optical birefringence measurements on 98% porosity silica aerogel samples subjected to various degrees of uniaxial compression up to 15% strain over a wide range of wavelength, 200 to 800 nm. Silica aerogels are composed of an entangled network of 3 - 5 nm diameter SiO2 strands and can be synthesized in a wide range of porosity, especially in the high porosity limit close to 99.9%, yet maintaining good mechanical stability. Uncompressed aerogels exhibit no or minimal degree of birefringence, indicating the isotropic nature of the material. Uniaxial compression of aerogel introduces global anisotropy, which produces optical activity in the material. We observed a quasi-linear strain dependence in |Δn| = |n_e - n_o| in compressed aerogels, where n_e(o) is the index of refraction for the extraordinary (ordinary) ray which has its polarization parallel to the compression axis. This effect has potential applications for aerogels as tunable waveplates operating in a broad spectral range.

1Support in part by NSF DMR-0803516 (YL) and DOE grant DE-FG02-02ER45984 (DT).

1:51PM Z26.00014 Microwave Absorption in Percolating Metal-insulator Composites1, DARIN ZIMMERMAN, JEREMY CARDELLINO, KYLE CRAVENER, KELLY FEATHER, NICHOLAS MISKOVSKY, GARY WEISEL, The Pennsylvania State University, Altoona — We measure several electromagnetic properties of tungsten-Teflon composites as a function of metal volume concentration. The electric (E) and magnetic (H) loss tangents at 2.45 GHz and the dc conductivity each exhibit a percolation transition at a different critical value of the metal volume fraction, p. Moreover, the transition behavior depends on the average particle size and size distribution of the metal component. We explain the variation in each case by a schematic model derived from established percolation theory and the distinct response of conducting particles to microwave electric and magnetic fields.

1This work was supported by grants from the National Science Foundation (NSF-RUI: DMR-0406584), The Pennsylvania State University, and Altoona College.
2:03PM Z26.00015 Anisotropy of induced polarization in the context of the generalized effective-medium theory.1, VLADIMIR BURMAN, Physics and Geophysics department, University of Utah, MICHAEL S. ZHDANOV2, Geophysics department, University of Utah, ALEXANDER GRIEBENKO, Geophysics Department, University of Utah — The rock samples are examples of heterogeneous complex structure material. Modeling of electromagnetic response of this medium makes it possible to study the anisotropy of induced polarization (IP) effect. The IP effect is studied in the context of the developed generalized effective-medium theory of induced polarization (GEMTIP). The effective-medium conductivity defined by the GEMTIP model, in a general case, is represented by a tensor function. This tensorial property of the effective-medium conductivity provides a new insight in the anisotropy phenomenon in the IP effect. As an example, we consider a multiphase composite polarized model of a rock formation with ellipsoidal inclusions. We demonstrate that the effective conductivity of this formation may be anisotropic, even if the host rock and all the grains are electrically isotropic.

1The authors acknowledge the support of the University of Utah Consortium for Electromagnetic Modelling and Inversion (CEMI)
2correspondent author

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Session Z27 GLMS: Advances in Instrumentation and Measurement II 329

11:15AM Z27.00001 ABSTRACT WITHDRAWN —

11:27AM Z27.00002 Surface Coatings for Gas Detection via Porous Silicon, SERDAR OZDEMIR, School of Physics, Georgia Institute of Technology, JI-GUANG LI, Nano Ceramics Center, National Institute for Materials Science, Japan, JAMES GOLE, School of Physics, Georgia Institute of Technology — Nanopore covered microporous silicon interfaces have been formed via an electrochemical etch for gas sensor applications. Rapid reversible and sensitive gas sensors have been fabricated. The fabricated porous silicon (PS) gas sensors display the advantages of operation at room temperature as well as at a single, readily accessible temperature with an insensitivity to temperature drift; operation in a heat-sunk configuration, ease of coating with gas-selective materials, low cost of fabrication and operation, and the ability to rapidly assess false positives by operating the sensor in a pulsed mode. The PS surface has been modified with unique coatings on the basis of a general theory in order to achieve maximum sensitivity and selectivity. Sensing of NH3, NO2, and PH3 at or below the ppm level have been observed. A typical PS nanostructure coated microstructured hybrid configuration when coated with tin oxide (NOx, CO) and gold nanostructures (NH3) provides a greatly increased sensitivity to the indicated gases. Al2O3 coating of the porous silicon using atomic layer deposition and its effect on PH3 sensing has been investigated. 20-100 nm TiO2 nanoparticles have been produced using sol-gel methods to coat PS surfaces and the effects on the selectivity and the sensitivity have been studied.

11:39AM Z27.00003 Directed-Assembly of Carbon Nanotubes on Soft Substrates for Flexible Biosensor Array1, HYOYUNG WOO LEE, JUNTAE KOH, BYUNG YANG LEE, TAE HYUN KIM, JOOYUNG LEE, SEUNGHI HONG, Department of Physics and Astronomy, Seoul National University, MIHYE YI, Korea Research Institute of Chemical Technology, YOUNG MIN JHON, Korea Institute of Science and Technology — We developed a method to selectively assemble and align carbon nanotubes (CNTs) on soft substrates for flexible biosensors. In this strategy, thin oxide layer was deposited on soft substrates via low temperature plasma enhanced chemical vapor deposition, and linker-free assembly process was applied onto the oxide surface where the assembly of carbon nanotubes was guided by methyl-terminated molecular patterns on the oxide surface. The electrical characterization of the fabricated CNT devices exhibited typical p-type gating effect and 1/f noise behavior. The bare oxide regions near CNTs were functionalized with glutamate oxidase to fabricate selective biosensors to detect two forms of glutamate substances existing in different situations: L-glutamic acid, a neuro-transmitting material, and monosodium glutamate, a food additive.

1The work was supported by the NRL, Seoul R&DB program and System IC 2010 grant.

11:51AM Z27.00004 Mid-infrared Verdet coefficient studies in GaAs, BaF2, and LaSrGaO3, and ZnSe, MYOUNG-HWAN KIM, Physics Dept., University at Buffalo, SUNY, VOLKER KURZ, Physics Dept., Universitaet Wuerzburg, GHEORGHE ACBAS, CHASE ELLIS, JOHN CERNE, Physics Dept., University at Buffalo, SUNY — We measure the mid-infrared (wavelength \( \lambda = 11 - 0.8 \mu m \); 0.1 - 1.5 eV) Faraday rotation and ellipticity in GaAs, BaF2, LaSrGaO3, and ZnSe. Since these materials are commonly used as substrates and windows in the mid-infrared, it is important to measure the Faraday signals for background subtraction and to test the accuracy of our measurement techniques. The light sources are lasers and a new custom-modified double-pass prism monochromator with a Xe lamp, which allowed continuous broadband measurements in the 0.31-1.5 eV energy range. Surprisingly, we find reproducible ellipticity signals, even though the radiation is well below the absorption edge of these materials and therefore no circular dichroism is expected. We suggest that the Faraday ellipticity is produced by the static retardance \( R_s \) of the ZnSe photoelastic modulator (PEM), which converts rotation signals into ellipticity. We determine \( R_s \) experimentally from the Faraday rotation and ellipticity ratio, produced by either applying a magnetic field or rotating the polarization of light incident on the PEM. Work supported by the Research Corp. Cottrell Scholar Award, NSF-CAREER-DMR0449899, and an instrumentation award from the CAS.

12:03PM Z27.00005 Diffraction by a Metallic Edge Near Plasma Frequency, MIGUEL A. ALVAREZ-CABANILLAS, National Polytechnic Institute, CITEDI — The behaviors of the fields diffracted by a metallic half-plane near plasma frequency are obtained. Incident plane wave with transverse magnetic polarization TM is diffracted by a gold sheet. The size of the atoms and the interatomic distance in the metallic sheet are assumed to be smaller than the wavelength. The electromagnetic field cannot detect the inner structure of the system and thus observes a medium conductivity defined by the GEMTIP model, in a general case, is represented by a tensor function. This tensorial property of the effective-medium conductivity provides a new insight in the anisotropy phenomenon in the IP effect. As an example, we consider a multiphase composite polarized model of a rock formation with ellipsoidal inclusions. We demonstrate that the effective conductivity of this formation may be anisotropic, even if the host rock and all the grains are electrically isotropic.

12:15PM Z27.00006 ABSTRACT WITHDRAWN —
These measurements show that the probe tips do not move with changing temperature and magnetic fields. To prevent materials from moving due to external vibrations, variable temperature magnetotransport measurements were performed. However, until this time a major inconvenience was caused by the thermal expansion of the probe tips and probe station as the temperature changed. To prevent movement, materials important for characterization and understanding of materials and devices are in use. Electrical and magnetic property measurements of nanoscale materials are important for characterizing and understanding of materials and devices. Equally important is to measure these properties at various temperatures.

In view of this, an optical system was constructed that closely simulates the Martian solar spectral irradiation, including seasonal variations due to the planet's orbit and attenuation by atmospheric dust. Upon exposure to this simulated environment, the OSL dating behavior of a suite of Martian sediment analogue materials were catalogued. Results suggest that the presence of the additional ionizing UV radiation on the surface of Mars will not compromise optical dating measurements of K- and Ca-feldspars, anhydrite, or hydrous Ca and Mg sulfates. However, Na-feldspar does appear to retain a trapped charge population, which could hinder optical dating of sediments containing more than trace amounts of sodic feldspars.

This work is supported by NSF-DMR-0602846.

12:39PM Z27.00008 The OSL dating behavior of Martian sediment analogue materials exposed to a simulated Martian solar spectrum. MARISSA DETSCH, Dept. of Physics, North Dakota State Univ., KEN LEPPER, Dept. of Geosciences, North Dakota State Univ. — Optically stimulated luminescence dating (OSL) is a terrestrial geochronometric technique being developed for in-situ dating of the geomorphic features on the surface of Mars. The solar spectral irradiance reaching the surface of Mars includes ionizing ultraviolet (UV) radiation that does not reach the surface of the Earth. In view of this, an optical system was constructed that closely simulates the Martian solar spectral irradiance, including seasonal variations due to the planet’s orbit and attenuation by atmospheric dust. Upon exposure to this simulated environment, the OSL dating behavior of a suite of Martian sediment analogue materials were catalogued. Results suggest that the presence of the additional ionizing UV radiation on the surface of Mars will not compromise optical dating measurements of K- and Ca-feldspars, anhydrite, or hydrous Ca and Mg sulfates. However, Na-feldspar does appear to retain a trapped charge population, which could hinder optical dating of sediments containing more than trace amounts of sodic feldspars.

12:51PM Z27.00009 ABSTRACT WITHDRAWN –

1:03PM Z27.00010 Variable temperature measurements in cryogenic probe stations; Measurements with Magnetic Fields. JEFFREY LINDEMUTH, Lake Shore Cryotronics — Electrical and magnetic property measurements of nanoscale materials are important for characterizing and understanding of materials and devices. Equally important is to measure these properties at various temperatures. These measurements are facilitated with cryogenic probe stations that provide a variable temperature environment over a wide range of temperatures. However, until this time a major inconvenience was caused by the thermal expansion of the probe tips and probe station as the temperature changed. To prevent movement from damaging the sample, the normal procedure is to lift the probe tips as the temperature changes. This prevents the implementation of totally automated variable temperature measurements. We present results using a new probe design that allows the probe tips to remain in contact to sample during temperature changes. With this new design we demonstrate, with optical microscopy, the total tip movement of less than 2 microns when the temperature of the sample changes from 4.2K to 300K. The same probes that eliminate the movement from thermal expansion also improve the isolation of the measurements to external vibrations. To show the performance of this probe design, variable temperature magnetotransport measurements were performed. These measurements show that the probe tips do not move with changing temperature and magnetic fields.

1:15PM Z27.00011 GHz-Bandwidth Signal Processing for Time-Resolved Faraday/Kerr Rotation Experiments1, YANJUN MA, PATRICK IRVIN, JEREMY LEVY — Faraday/Kerr rotation is a sensitive measurement of the electron spin and its dynamics in semiconductor nanoscale devices such as GaAs quantum dots. The Kerr rotation angle from a single spin, however, can be as small as 10^-6 rad, which requires massive averaging of the Kerr signal in order to maximize the signal-to-noise ratio. By replacing the mechanical delay line typically found in time resolved Kerr rotation (TRKR) measurements with a continuous wave probe and high-speed electronics, the signal and noise can be sampled more often which results in a higher SNR. However, real-time methods for data collection are typically limited by available memory, resulting in unavoidable dead time for which data cannot be collected and averaged. The approach we have developed integrates a field-programmable gate array (FPGA) with a high-speed digitizer, thus allowing high-speed on-board averaging to overcome these technical limitations. We will demonstrate the performance of this instrument by comparing the results of this study with traditional pump-probe (sampling) techniques and discuss its applicability for a variety of dynamical spin-sensitive experiments in the solid state.

This work is supported by NSF-DMR-0602846.

11:15AM Z28.00001 Fundamental Etching and Roughening Mechanisms of Photoresist Polymers during Plasma Processing, DUSTIN NEST, TING-YING CHUNG, DAVID GRAVES, UC-Berkeley Dept. of Chemical Eng., FLORIAN WEILNOECKER, ROBERT BRUCE, TSUNG CHENG LIN, RAY PHANEUF, GOTTFRIED OEHRLEIN, University of Maryland, College Park, ERIC HUDSON, Lam Research Corp., DEYAN WANG, CECILY ANDES, Rohm and Haas Electronic Materials — Reducing the etching and roughening of photoresist polymers during plasma processing is required as optical lithography for integrated circuit manufacture is extended to patterning features with critical dimension control on the order of nanometers. We use a vacuum beam system to simulate plasma exposure but under well-defined conditions. Samples are exposed to well-characterized beams of ions, vacuum ultraviolet (VUV) radiation, and electrons under high vacuum conditions. Post-exposure analysis includes atomic force and scanning electron microscopy and FTIR spectroscopy. We show that VUV radiation, ion bombardment, the ion / photon flux ratio and heating all play a role in the roughening of current-generation PMMA-based 193 nm photoresists. VUV radiation breaks carbon-oxygen bonds to a depth of approximately 100 nm whereas ion bombardment forms a dehydrogenated surface layer. Qualitatively similar roughening was observed in plasmas with the same ion bombardment energy and ion and VUV fluence.

11:27AM Z28.00002 Understanding the Differences between Electron and Ion Guiding, SUSANTA DAS, BUDDHIKA S. DASSANAYAKE, JOHN A. TANIS, Western Michigan University, NIKOLAUS STOLTERFOHT, Helmholtz-Zentrum Berlin, ATOMIC PHYSICS GROUP TEAM — Significant differences in the transmission and guiding of slow positive ions and fast electrons through insulating PET nanocapillary foils have been observed.1,2 While ions are transmitted without energy loss or change in charge state even when the foil is tilted with respect to the incoming ion beam, electrons undergo inelastic as well as elastic scattering leading to considerable reduction in the transmitted intensities. The underlying reasons for the differences between ions and electrons will be discussed and quantitative comparisons made. Qualitatively, slow positive ions are fully neutralized when striking a surface and consequently deposit all of their charge, whereas electrons can be elastically or inelastically scattered.3 Additionally, secondary electron emission by incident ions increases the deposited charge, while this same emission decreases the deposited charge for electrons. *Supported by Research Corporation 1N. Stolterfoht et al., Phys. Rev. A 77, 032905 (2008). 2S. Das et al., Phys. Rev. A 76, 042716 (2007). 3B. Stix et al., XXV ICPEAC, Freiburg, Germany, July 2007, Abstracts, MO 128.
11:39 AM Z28.00003 Laser Manipulation of Nanostructures, DINKO CHAKAROV, Chalmers University of Technology — This work describes a new method for controlling the pattern into which nanoparticles in a disordered metal-nanoparticle layer organize themselves by a single light pulse. The phenomena behind formation of one- and two-dimensional grating patterns are attributed to interference effects between the incident light and waveguided modes. Such self-patterning behavior could be useful for the fabrication of complex nanostructures and advanced phononic devices.


1This work was partly supported through Swedish Foundation for Strategic Research program PHOTO/NANO.

11:51 AM Z28.00004 A new method of nano-manipulation with AFM derived from nanotribology, SUENNE KIM, Department of Physics, University of Texas at Austin, DANIEL RATCHFORD, XIAOQIN LI — Based on principles of nanotribology, a new approach is explored for manipulating nanoparticles (ranging from 5nm to 60nm in diameter) with an Atomic Force Microscope (AFM). In this new approach, one first kicks a nanoparticle. Immediately following the kicking event, static friction is greatly reduced. One can then dribble the nanoparticle to the desired position in the tapping (imaging) mode of the AFM. The major advantage of this scheme lies in the active manipulation with simultaneous visual feedback. Our study revealed the mechanism for the nano-displacement is primarily governed by the “stick” events of the stick-slip process. We also found that the manipulation can be effectively controlled by adjusting the scanning speed, and the critical speed depends on the local roughness of the surface.

1This research is supported by NSF DMR-0747822, NSF-IGERT, Welch Foundation grant F-1662 and ONR grant N00014-08-1-0745.

12:03 PM Z28.00005 Single-Particle Placement on a large scale, PRADEEP BHADRACHALAM, HONG-WEN HUANG, VISHVA RAY, SEONG JIN KOH, University of Texas at Arlington — The capability of positioning single nanoparticles onto exact substrate locations holds prime technological and scientific importance. We present a novel technique to precisely place exactly one single nanoparticle onto a targeted substrate location on a large scale. This was done by defining an electrostatic guiding structure using CMOS compatible fabrication technology, which guides exactly one single 20nm gold nanoparticle onto a desired substrate location with a success rate over 90%. The measured precision of this single-particle placement (SPP) was 12.1nm. This technique has an inherent capability of limiting one single nanoparticle for each target location. Theoretical calculations has revealed that this self-limiting capability originates from an increased free energy barrier after a nanoparticle is placed on the target location, effectively blocking the approach of other nanoparticles. We also demonstrate size-selective placement of single nanoparticles, where individual nanoparticles of different sizes are guided to different target locations on the same substrate.

1(Supported by: NSF-CAREER(ECS-0449958), ONR(N00014-05-1-0050), THECB(003656-0014-2006))

12:15 PM Z28.00006 Magnetically Driven Swimming of Nanoscale Colloidal Assemblies, JENNIFER BREIDENICH, JASON BENKOSKI, LANCE BAIRD, RYAN DEACON, H. BRUCE LAND, ALLEN HAYES, Milton S. Eisenhower Research Center, The Johns Hopkins University Applied Physics Laboratory, Laurel MD 20723, PEI KENG, JEFFREY PYUN, Department of Chemistry, University of Arizona, Tucson AZ 85721 — At microscopic length scales, locomotion can only be generated through asymmetric conformation changes, such as the undulating flagellum employed by protozoa. This simple yet elegant design is optimized according to the dueling needs of miniaturization and the fluid dynamics of the low Reynolds number environment. In this study, we fabricate nanoscale colloidal assemblies that mimic the head + tail structure of flagellates. The assemblies consist of two types of magnetic colloids: 25 nm polystyrene-coated Co nanoparticles, and 250 nm polyethylene glycol coated magnetite nanoparticles. When mixed together in N-dimethylformamide, the Co nanoparticles assemble into flexible, segmented chains ranging in length from 1 - 5 µm. These chains then attach at one end to the larger magnetic beads due to magnetic attraction. This head + tail structure aligns with an external uniform magnetic field and is actuated by an oscillating transverse field. We examine the effects of Co nanoparticle concentration, magnetite bead concentration, magnetic field strength, and oscillation frequency on the formation of swimmers and the speed of locomotion.

12:27 PM Z28.00007 Observation of Fano Interference and Field Dependence by Raman Spectroscopy of Molecularly Doped Silicon, BRIAN BURKE, KEITH WILLIAMS, JACK CHAN, University of Virginia — We have investigated various doping techniques on silicon to form thin, highly p-doped layers near the surface (approximately 10 nm). We are able to observe through Raman spectroscopy the signature Fano lineshape present in the zone-centre optical phonon. We have defined high resolution channels by electron beam lithography and subsequently annealed adsorbed dopant molecules into the silicon lattice by RTA. We have performed sheet resistance measurements as well as Raman mapping to characterize the doping profile. The Raman laser line of 325 nm provides a penetration depth of roughly 8 nm, ideal for studying the surface of silicon. After studying the highly doped channel, electrodes were deposited and field dependence measurements were made. Additionally, IETS and transport measurements have been conducted for various geometries to compare with Raman data.

12:39 PM Z28.00008 Profiling surfaces with a carbon nanotube oscillator, ADRIAN POPESCU, LILIA WOODS, University of South Florida, IGOR BONDAREV, North Carolina Central University — A practical device for profiling surfaces is proposed, as an alternative to an Atomic Force Microscopy (AFM) tip. The device consists of a finite length double wall carbon nanotube oscillator with the outer tube being stationary and oriented perpendicular to the surface plane. By investigating the changes in the oscillatory behavior of the inner tube due to the proximity of the surface, the roughness of the surface can be determined. The role of the length and the initial extrusion of the moving tube, and the friction losses in the motion process are also explored. We suggest that such a device can be virtually a non-fatigue, non-wear system, and that it is possible to obtain a higher in-plane resolution as compared to the “traditional” AFM tip.

1DE-FG02-06ER42197

12:51 PM Z28.00009 An Electrodynamics Ratchet Motor, JIUFU LIM, University of Melbourne, School of Chemistry, JOHN SADER, University of Melbourne, Department of Mathematics and Statistics, PAUL MULVANEY, University of Melbourne, School of Chemistry — Brownian ratchets are often used to generate translational motion for biological separation processes and colloidal transport. This talk will propose a Brownian ratchet motor that enables the transduction of electrical energy into rotary micro-mechanical work. This is achieved through torque generation provided by boundary shaping of equipotential surfaces. Stochastic simulations elucidate the performance characteristics of this device as a function of its geometry. Miniaturization to nanoscale dimensions yields rotational speeds in excess of 1kHz, which is comparable to biomolecular motors of similar size.

1Australian Research Council Grants Scheme, Albert Shimmins Fund
investigated, for the new germanium/cobalt co-substituted cobalt ferrite Co

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A rigid band picture is proposed to estimate the trend of magnetostrictive coefficients of Fe, Ga and Zn compounds. Although the rare earth-3d metal compound, such like TbFe2, have large positive magnetostriction of

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The magneto-crystalline anisotropy energy

calculations, we have investigated the Young's modulus, shear modulus, anisotropy energy and magnetostriction of Ga, Al, Zn, Ge and Be doped in bulk Fe. In fact doping some nonmagnetic element, such as Ga, Al, Zn and Be, strongly alters the anisotropy energy and enhances the magneticostiction, which indicated

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= 0 - 5 T. The high field regions of these loops were then fitted to the Law of Approach to Saturation (LA) for cubic materials as given by

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165319 (2005).

MCA

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with high magnetostrictive materials with low material costs. Nanocrystalline Fe-based alloys without rareearths are very interesting candidates due to the

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1

1

< 0.20 heat-treated to increase the magnetostriction that is otherwise absent. This diffuse scattering exhibits asymmetric peaks at the (100) and (300) reciprocal lattice positions that are consistent with the coexistence of short-range ordered, coherent nanoprecipitates embedded in a long-range ordered, body-centered cubic matrix. A large peak splitting is observed at (300) for x=0.19, which suggests that the nanoprecipitates are not cubic but have a lower symmetry and a large elastic strain. The strongest diffuse scattering occurs for x=0.19 where the maximum magnetostriction is found. This suggests a structural origin for the enhanced magnetostriction in these materials.

This research was sponsored by the Office of Naval Research under Grant MURI N00014-06-1-0530, and N00014-06-1-0204.

This work was supported by the UK EPSRC under grant number EP/D057094 and by the US NSF under grant number DMR-0402716.

1Work is supported by US DOE (Grant No. DEFG02-05ER46237).

11:39AM Z28.00010 When a magnetized quantum wire can act as an “active” laser medium

, MANVIR KUSHWAHA, University of Puebla, Mexico — We report on the theoretical investigation of magnetoplasmon excitations in a quantum wire characterized by a confining harmonic potential and in the presence of a perpendicular magnetic field. The problem involves two length scales: l_0 = \sqrt{\hbar/\mu_0 \omega_0} and l_\perp = \sqrt{\hbar/m^* \omega_\perp}, which characterize the relative strengths in the interplay of confinement and the magnetic field. We embark on the charge-density excitations within a two-subband model in the framework of Bohm-Pines’ random-phase approximation. The main focus of our study is the (intersubband) magnetoroton excitation which changes the sign of its group velocity twice before merging with the respective single-particle continuum. We analyze the terms and conditions within which the magnetoroton excitation persists in the quantum wires. It is suggested that the electronic device based on such magnetoroton modes can act as an active laser medium.

11:39AM Z28.00011 Suppression of electric field domains in semiconductor superlattices with side shunting layer

1. HUIDONG XU, Duke University, ANDREAS AMANN, Tyndall National Institute, Ireland, ECKEHARD SCHÖLL, Technical University of Berlin, Germany, STEPHEN TEITSWORTH, Duke University — We have numerically studied the electronic transport properties of a weakly-coupled semiconductor superlattice that possesses a conductive side shunting layer, using a model that includes lateral dynamics in each quantum well of the superlattice [1]. Depending on the lateral size of the superlattice quantum wells and the quality of the connection between the shunt layer and the superlattice, the shunt may inhibit the formation of electric field domains in the superlattice under conditions of negative differential resistance (NDR). We determine conditions to achieve a stable spatially-uniform electric field distribution, an important condition for practical NDR devices such as superlattice THz oscillators. For a superlattice with small lateral extent, a high quality shunt stabilizes the uniform field configuration in the entire structure, whereas a lower quality shunt leads to current oscillations and/or static field domains. We characterize the bifurcations associated with the transitions between these different behaviors. [1] A. Amann and E. Schöll, Phys. Rev. B 72, 165319 (2005).

Friday, March 20, 2009 11:15AM - 1:27PM – Session Z29 GMAG: Magnetostructural Effects and General Magnetism

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11:15AM Z29.00001 Non-cubic, coherent nanoprecipitates observed by neutron diffuse scattering in highly magnetostrictive Galfenol (Fe1−xGax) alloys.

1. PETER GEHRING, National Institute of Standards and Technology, HU CÃO, CHRIS DEVREUGD, Virginia Tech, JOSE ABELARDO RODRIGUEZ, University of Maryland, JIE FANG LI, DWIGHT VIEHLAND, Virginia Tech — We report neutron diffuse scattering measurements on highly magnetostrictive Fe1−xGax alloys with different thermal treatments. Diffuse scattering is seen for compositions 0.14<x<0.20 heat-treated to increase the magnetostriction that is otherwise absent. This diffuse scattering exhibits asymmetric peaks at the (100) and (300) reciprocal lattice positions that are consistent with the coexistence of short-range ordered, coherent nanoprecipitates embedded in a long-range ordered, body-centered cubic matrix. A large peak splitting is observed at (300) for x=0.19, which suggests that the nanoprecipitates are not cubic but have a lower symmetry and a large elastic strain. The strongest diffuse scattering occurs for x=0.19 where the maximum magnetostriction is found. This suggests a structural origin for the enhanced magnetostriction in these materials.

1Supported in part by NSF grant DMR-0804232.

11:27AM Z29.00002 Magnetic and magnetoelastic properties of Ge/Co co-substituted cobalt ferrite

1. NARESH RANVAH, EUGENE MELIKHOV, JOHN SNYDER, DAVID JILES, Wolfson Centre for Magnetics, Cardiff University, WOLFSON CENTRE FOR MAGNETICS TEAM — The highly magnetostrictive material cobalt ferrite and its derivatives based on substitution of cations have been shown to have extreme sensitivity of their magnetization to stress. In order to control their properties (e.g. magnetostriction, magnetic anisotropy, strain derivative, and hysteresis) substitution of specific cations are needed. We have shown Ge1/4/Co3/4 co-substituted cobalt ferrites (Co1.25+Ge0.25Fe0.75O4) to have very interesting combinations of magneto-elastic properties. In the present study the variation of magnetic anisotropy with composition and temperature was investigated, for the new germanium/cobalt co-substituted cobalt ferrite Co1+x,GexFe2−x,O4. Hysteresis loops were measured in the range T = 10 - 400 K, with μHmax = 0 - 5 T. The high field regions of these loops were then fitted to the Law of Approach to Saturation (LA) for cubic materials as given by M = M_s[1-(8/105)(K1/\mu_0 M_s H)^2], plus a linear forced magnetisation term. Values for first order cubic anisotropy constant K1 were calculated and it was found that anisotropy increased as temperature decreases for all compositions. At most temperatures anisotropy decreased with increase in x.

1Supported by US DOE (Grant No. DEFG02-05ER46237).

11:39AM Z29.00003 Magnetostriction of Fe-based alloy

1. YANNING ZHANG, JUEXIAN CAO, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, California, 92697 USA — High magnetostrictive materials are important for sensor and actuator applications. Although the rare earth-3d metal compound, such like TbFe2, have large positive magnetostriction of ~2600ppm, their practical application was hindered due to larger activation external magnetic field and their high material costs. Large-scale industrial applications require soft magnetic materials with high magnetostrictive materials with low material costs. Nanocrystalline Fe-based alloys without rareearths are very interesting candidates due to the fact doping some nonmagnetic element, such as Ga, Al, Zn and Be, strongly alters the anisotropy energy and enhances the magnetostriction, which indicated substituting Fe by nonmagnetic elements might be a new method to develop cheap and soft magnetic material with high magnetostriction. With First-principle calculations, we have investigated the Young’s modulus, shear modulus, anisotropy energy and magnetostriction of Ga, Al, Zn, Ge and Be doped in bulk Fe. The magneto-crystalline anisotropy energy E_{JC,4} and the magnetostrictive coefficients (λ_{M4}) strongly depend on the compositions and atomic arrangement. A rigid band picture is proposed to estimate the trend of magnetostrictive coefficients of Fe, Ga and Zn compounds.

1Work is supported by US DOE (Grant No. DEFG02-05ER46237).
11:51AM Z29.00004 The Magnetocaloric Effect in Single Crystal and Processed Polycrystalline MnP\footnote{Work supported by DOE grant #DE-FG02-08ER46481.}, RYAN A. BOOTH, SARA A. MAJETHI, Carnegie Mellon University — Manganese Phosphide (MnP) is a promising magnetocaloric effect (MCE) material for use in room temperature-magnetic refrigeration because it exhibits a first-order ferromagnetic to paramagnetic phase transition at a Curie temperature of 290 K, possesses no measurable magnetic hysteresis, and has a saturation field of lower than 7.5 kOe along the c-axis. The magnetic entropy change ($\Delta S$) was measured in single crystals along the c-axis to be 2.2, 3.3, and 6.0 J / kg K in applied fields of 10 kOe, 20 kOe, and 50 kOe respectively. Cold-rolling followed by a short annealing of polycrystalline MnP was shown to create preferential crystallographic alignment that mimics the favorable properties of single crystals without the expenses associated with their growth. A comparison of the magnetocaloric effect between single crystals and rolled polycrystalline MnP is presented.

12:03PM Z29.00005 Magnetic anisotropy dependency on structural properties in strained MnAs thin films, MAGNUS WIKBERG, Dep. Eng. Sciences, Uppsala University, MIKAEL OTTOSON, Dep. Materials Chemistry, Uppsala University, JANUSZ SADOWSKI, MAX-Lab, Lund University, RONNY KNUST, OLOF KARIS, Dep. Physics and Materials Science, Uppsala University, PETER SVELLINDH, Dep. Eng. Sciences, Uppsala University — High quality thin films of MnAs (between 30 and 200 Å) have been grown with molecular beam epitaxy (MBE) on GaAs(111)B and (001) substrates and under different growth conditions. The magnetic anisotropy of the MnAs layers has been investigated with SQUID magnetometry and magnetic force microscopy (MFM). A clear correlation between choice of substrate, growth temperature and film thickness can be seen in the magnetic anisotropy and $T_c$ measurements with a rapid transition towards bulk like anisotropy constants as the film thickness is increased. From X-ray diffraction, a relationship between $T_c$ and lattice strain has been established, where the film with increasing film thickness rapidly exhibits a transition from a highly strained to a fully relaxed film. A complex dependence on the structural transition from the ferromagnetic to the paramagnetic phase is also seen in X-ray magnetic circular dichroism (XMCD) measurements, where the orbital moment does not strictly follow the spin moment near the ferromagnetic-paramagnetic phase transition.

12:15PM Z29.00006 Coercivity of Melt-Spun Gd$_{100-x}$Fe$_x$\footnote{Funded by NSF Grants Nos. DMR-0504177 and DMR-0504706}, PAUL SHAND, ANDREW MEYER, University of Northern Iowa, DAVID SCHMITTER, Providence College, GEOFFREY ROJAS, JEFFREY SHIELD, JARED GOERTZEN, University of Nebraska-Lincoln, DANIAL HASKEL, Argonne National Laboratory, DIANDRA LESLIE-PELECKY, University of Texas at Dallas — We have measured the coercivity of melt-spun Gd$_{100-x}$Fe$_x$ (0 \leq x \leq 50) alloys over the temperature range 2 K \leq T \leq 340 K. Previously performed structural measurements revealed that the system consists of crystalline hcp-Gd grains surrounded by a non-crystalline Gd or Gd-Fe phase composed of $\text{Gd}_{25-y} \cdot \text{Fe}_y$, where $x > y$ is the iron concentration in the amorphous region. The two-phase structure is responsible for an unusual dependence of the coercivity on temperature in which non-zero coercivity is observed above the hcp-Gd $T_c$ with a peak near 320 K. The coercivity decreases as the hcp-Gd grains order, then increases with decreasing temperature. This behavior is explained by the presence of Fe-rich magnetically correlated regions.

12:27PM Z29.00007 ABSTRACT WITHDRAWN —

12:39PM Z29.00008 Epitaxial growth and spin dependent states of Co$_2$Mn$_x$Si$_{1-x}$ (111) thin films\footnote{The work is supported by DOE BES DE-FG02-05ER46216 and NSF DMR-0441218.}, LIANG HE, BRIAN COLLINS, FRANK TSUI, University of North Carolina at Chapel Hill, YONG CHU, APS, Argonne National Laboratory — Epitaxial growth of Co$_2$Mn$_x$Si$_{1-x}$ on Ge (111) substrates has been studied using combinatorial MBE techniques, including that of the Heusler alloy Co$_2$MnSi. For Si concentration of 25 at. \%, in-situ RHEED and ex-situ X-ray diffraction experiments indicate that the epitaxial growth is coherent for atomic ratio Co:Mn between 1 and 9, while the film is microcrystalline for Co:Mn < 1 and it is rough and of poor crystalline quality for Co:Mn > 9. The crystalline quality is the highest around Co:Mn = 4, whereas it exhibits a plateau around a ratio of 2, i.e. the Heusler alloy, Co$_2$MnSi. Within the region of coherent growth, at coverages below 100 Å, the growth front is smooth and 2D-like. As thickness increases, the surface morphology systematically changes from quasi-2D into 3D. The morphology transition also depends sensitively on composition, i.e. Co:Mn ratio, and temperature. Spin-dependent states as a function of composition at low coverages have been examined by tunneling spectroscopy using Al$_2$O$_3$ as the tunneling barrier and Fe and Nb as the detector layers.

12:51PM Z29.00009 Self-energy of half-metallic ferromagnet Mn$_x$Si$_{3-x}$ calculated from infrared spectroscopy data, S.V. DORDEVIC, The University of Akron, N. STOJILOVIC, John Carroll University, L.W. KOHLMAN, The University of Akron, C. PETROVIC, Brookhaven National Laboratory — We will report the results of our infrared and optical spectroscopy study of a half-metallic ferromagnet Mn$_x$Si$_{3-x}$. This compound is currently being investigated as potential injector of spin polarized currents into germanium. Infrared measurements have been performed over a broad frequency (30 - 50000 cm$^{-1}$) and temperature (10 - 300 K) range. From the complex optical conductivity $\sigma(\omega)$ we extract the electron self-energy $\Sigma(\omega)$. The calculation of $\Sigma(\omega)$ is based on novel numerical technique which uses Lvenberg–Marquardt algorithm for solution of systems of non-linear equations. Obtained self-energy provides a new insight into electron correlations in Mn$_x$Si$_{3-x}$.

1:03PM Z29.00010 Electronic and Magnetic properties of Transition Metal Borides, ADITI HERWADKAR, National Renewable Energy Laboratory, YUFENG ZHAO — Boron has three valence electron and a small covalent radius undergoing sp$_2$ hybridization in many boron clusters. It is also known to form large variety of crystal structures both planar and 3D caged molecules. Our current work is to study transition metal boride clusters. This would be useful towards designing metal boride nanoclusters with tunable optical, magnetic and electron transport properties. Different stoichiometries are studied. The metal to Boron ratio varies from 0.3 to 0.75. For each of these compositions the lowest energy geometries were determined by optimizing the bond length for several initial symmetric geometries. The lowest energy structure is then chosen as the equilibrium structure. Most strikingly, all these transition-metal boride clusters are cage-like although both boron and transition metal usually favor high coordination number. We also find that some of the clusters have an extremely high magnetic moment per unit mass. This renders metal boride nanoparticles as potentially promising light-weighted magnetic materials. All the calculations are done using the spin-polarized density functional theory method implemented in the Vienna ab initio simulation package. A plane wave basis set with (400 eV cutoff) was used in combination with an all electron like projector augmented wave potential and PBE exchange correlation functional with in the generalized gradient approximation.
1:15PM Z29.00011 Revisiting Classical Diamagnetism: A Surprise of Physics, NARENDR A KUMAR, Raman Research Institute, VIJAY KUMAR KRISHNAMURTHY, Indian Institute of Science — The Classic Bohr-van Leeuwen (BvL) theorem states that the orbital diamagnetism of a classical system of charged particles in thermal equilibrium is identically zero. This theorem is universally accepted and has entered textbooks. Physically, the theorem derives from the exact cancellation of the orbital diamagnetic moment associated with the completed cyclotron orbits of the charged particles by the paramagnetic moment subtended by the incomplete orbits skipping the boundary cuspidally in the opposite sense. In this work we have revisited the problem of this crucial but subtle role of the boundary by considering the case of a finite but unbounded system, namely that of a charged particle moving on a sphere in the presence of an externally applied magnetic field. The orbital moment calculated on the basis of the classical Langevin equation in the infinite time limit now indeed turns out to be non-zero, and has the diamagnetic sign. This violates the BvL theorem as stated in the literature. To the best of our knowledge, this is the first report of non-zero classical diamagnetism. It is explicitly owing to the above avoided cancellation. We also present possible experimental realization of the predicted classical diamagnetism.


11:15AM Z30.00001 Multiferroic states in perovskite type orthoferrites, YUSUKE TOKUNAGA, ERATO-JST, SATOSHI IGUCHI, The Univ. of Tokyo, YASUJIRO TAGUCHI, CMRGC, RIKEN, TAHAKISA ARIMA, Tohoku Univ., YOSHINORI TOKURA, ERATO-JST, The Univ. of Tokyo, CMRGC, RIKEN — Versatile and gigantic magneto-electric (ME) phenomena have been found for a single crystal of perovskite-type orthoferrite DyFeO$_3$. Below the antiferromagnetic ordering temperature of Dy moments, a linear ME tensor component as large as $a_{xx} \sim 2.4 \times 10^{-2}$ in dimensionless CGS unit is observed. In addition, it is revealed that the application of magnetic field along the c axis induced a ferroelectric order whose large polarization ($\geq 0.2 \mu$C/cm$^2$ along the c-axis) can be directly reversed by either of magnetic field or electric field. It is noteworthy that this magnetically driven ferroelectric state is even weakly ferromagnetic, i.e., truly multiferroic, in nature. We propose here that the exchange striction working between adjacent Fe$^{3+}$ and Dy$^{3+}$ layer with the respective layered antiferromagnetic components can be the origin of the ferroelectricity with such a large polarization value. It is further argued that the reversal process of electric polarization by magnetic (electric) field is inherently related to the change of the relative phase of antiferromagnetic spin (moment) arrangement of Fe (Dy) [1].


11:27AM Z30.00002 Composite Domain Walls in Multiferroic Orthoferrites RFeO$_3$, NOBUO FURUKAWA, Dept. of Physics, Aoyama Gakuin Univ. and ERATO-Multiferroics, JST, HOSHO KATSURA, CMRGC, RIKEN — In order to analyze novel magneto-electric effects such as electric-field controlled magnetization-flips in multiferroic orthoferrites RFeO$_3$, we study an effective model which includes d-spins on Fe sites and f-spins on R sites. Order parameters for d and f spins are coupled through Peierls distortions. Ginzburg-Landau theory is applied to investigate domain wall structures of the model. As a result, we find various types of solitons corresponding to ferromagnetic, ferroelectric and composite ferromagnetic-ferroelectric domain walls. Dynamics of the domain walls under external fields will also be presented.

11:39AM Z30.00003 Multiferroic BiFeO$_3$, SANG-WOOK CHEONG — BiFeO$_3$ (BFO) is a unique multiferroic in the sense that the magnitude of ferroelectric polarization is large (about 90 microC/cm$^2$) - similar with that of standard ferroelectrics such as BaTiO$_3$ and PbTiO$_3$. In addition, both magnetic and ferroelectric temperatures are much high than room temperature. BFO has been extensively studied, but mostly in the form of films. In order to explore the intrinsic properties of BFO and also properties that cannot be measured in film forms, we have investigated comprehensive physical properties of bulk BFO single crystals using a number of techniques such as neutron scattering, piezoelectric force microscopy and transport property measurement.

11:51AM Z30.00004 Polarized Neutron Investigations of BiFeO$_3$, WILLIAM RATCLIFF, NIST, SEONGSU LEE, TAEKJIB CHOI, Department of Physics, Rutgers University, ROSS ERWIN, NIST, SANG WOOK CHEONG, VALERY KIRYUKHIN, Department of Physics, Rutgers University — BiFeO$_3$ is a multiferroic material at room temperature. Until recently, the only studies on this material were performed on either thin films or powders. We report on the results of neutron diffraction studies performed on single crystals of BiFeO$_3$. Polarized neutron diffraction results unambiguously reveal that the magnetic structure of this material is chiral. Furthermore, neutron diffraction experiments have shown that it is possible to control magnetic domain populations through the application of an external electric field. These results may suggest directions for future research performed in thin films.

12:03PM Z30.00005 Weak ferromagnetism in a high-pressure phase of FeTiO$_3$ with polar lattice distortion, TAMAS VARGA, JOHN MITCHELL, Argonne National Laboratory, CRAIG FENNIE, Cornell University, STEPHEN STREIFFER, SEUNGBUM HONG, MOONKYU PARK, Argonne National Laboratory, VENKATRAMAN GOPALAN, AMIT KUMAR, EFTHTIA VLHOS, Pennsylvania State University, TAKESHI SANEHIRA, YANBIN WANG, University of Chicago — Today’s challenge in multiferroics is to identify materials in which polarization and magnetization – normally considered contraindicated properties - are strongly coupled. Recent density functional theory calculations have predicted that the family of compounds MFeO$_3$ ($M = Mn$, Fe, Ni) are promising candidates where a polar lattice distortion can induce weak ferromagnetism. The crucial insight is that while the equilibrium one-atmosphere structure of these is ilmenite, they must be transformed to a closely related LiNbO$_3$-type structure. We have corresponded the FeTiO$_3$ phase at 18 GPa and 1200 °C. It shows a sharp antiferromagnetic (AF) transition at 111.5 K. FeTiO$_3$ also displays ferroelectric domains, and weak ferromagnetism coincident with the AF transition. Possible coupling between its polarization and weak ferromagnetism is discussed based on results of piezoelectric force microscopy (PFM), second harmonic generation (SHG), dielectric, and polarization measurements.

3 The work at Argonne National Laboratory, including the use of the Advanced Photon Source, was supported by the U.S. DOE Office of Science, Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

12:15PM Z30.00006 EXAFS Studies of Multiferroic Pb(Ti,Fe)O$_3$, YING ZOU, SOMADITYA SEN, SHISHIR RAY, MARK WILLIAMSEN, University of Wisconsin-Milwaukee, USA, TOMOHIRO SHIBATA, SOMA CHATTOPADHYAY, Illinois Institute of Technology, USA, MALI BALASUBRAMANIAN, APS-Argonne National Laboratory, USA, PRASENJIT GUPTASARMA, University of Wisconsin-Milwaukee, USA — Recent suggestions [1] of multiferroic behavior in Pb(Ti,Fe)O$_3$ has revived an interest in this text-book ABO$_3$ type ferroelectric material. Here, we study the effect of Fe-substitution on the local structural and chemical environment of the parent PbTiO$_3$ phase. We have carried out extended x-ray absorption fine structure (EXAFS) measurements at the Fe-K, Ti-K and Pb-LIII edge at the Advanced Photon Source, on a series of single phase samples of PbTi$_{1-x}$Fe$_x$O$_3$ ($0 < x < 0.5$) synthesized using a sol-gel technique. The near edge fine structure (XANES) reveals that Fe cations are trivalent. A fascinating new result is the observation of charge disproportionation of Pb into Pb2+ and Pb4+, likely a result of charge redistribution arising from Fe3+ substitution. Radial distribution function (RDF) study of EXAFS spectra from the Ti-K edge and the Fe-K edge confirms that Fe substitutes Ti up to x=0.5. 1. Palmer et al, Appl. Phys. Lett. 90(2007)172901.

3 Corresponding author
12:27PM Z30.00007 Phase formation, Crystal Lattice and Microstructure Studies of sol-gel derived Pb(Ti,Fe)O$_3$. SOMADITYA SEN, DAVID GELTING, SHISHIR RAY, YING ZOU, DONALD ROBERTSON, MARIJA GAJDARDZIKA-JOSIFOVSKA, LARRY BUROKER, MARK WILLIAMSEN, PRASENJIT GUPTASARMA$^2$. Physics Dept., Univ. of Wisconsin, Milwaukee, 1900 E Kenwood Blvd, Milwaukee, WI 53211, USA — It has recently been suggested$^1$ that Fe-substituted PbTiO$_3$ can exhibit magnetoelectric multiferroic behavior. With an intent to examine whether Fe can fully substitute the lattice in Pb(Ti,Fe)O$_3$ and to study its effect on crystal structure, we have synthesized highly phase pure nanopowders from citric acid metal ion chelate complexes stabilized by glycercoll in a sol gel. Using variety of probes, we demonstrate that Fe can substitute Ti up to at least 0.5 atoms per formula unit of Pb(Ti,Fe)O$_3$. Rietveld refinement of XRD data, from both laboratory and synchrotron sources, demonstrates that crystal structure of Fe substituted phases can be derived from the parent orthorhombic PbTiO$_3$ phase. Increasing concentration of Fe up to $x=0.3$ results in drastic change in lattice parameters and decrease in orthorhombic distortion. These results are supported by detailed studies of XRD, TEM and XAFS.

2. NSF, RGI
3.correspondence: pg@uwm.edu

12:39PM Z30.00008 Electric polarization and magneto-dielectric effect in charge ordered system with frustrated geometry. TSUTOMU WATANABE, IMRAM, Tohoku University, SUMIO ISHIHARA COLLABORATION — Recently discovered multiferroic materials, where electric polarization and non-collinear spin structure coexist, are recognized as ferroelectric materials driven by spin ordering. There is another class of ferroelectricity where the electric polarization is attributed to the electronic charge ordering. Layered iron oxide LuFe$_2$O$_4$ belongs to this class of material. Ferroelectric transition occurs at almost the same temperature with the charge ordering one where Fe$^{1+}$ and Fe$^{3+}$ are aligned in the paired triangular lattices. Therefore, it is expected that the frustration plays important roles on breaking of the space inversion symmetry. We study theoretically a possibility of the charge-driven ferroelectric transition, and, in particularly, focus on the electron quantum transfer effects. We analyzed the V-t model, where t and V are the transfer integral and the Coulomb repulsion between nearest-neighbor sites, respectively, by using the variational Monte Carlo method. We found that the quantum fluctuation and frustration tend to enhance the stabilization of a three-fold charge ordered state and electric polarization although the polarization is small. In addition, we studied the effect of the spin ordering. It is found that, in some spin ordered structures, the electric polarization is stabilized accompanying the three-fold charge orderd state.

12:51PM Z30.00009 Charge order, dynamics, and magneto-structural transition in multiferroic LuFe$_2$O$_4$. XIAOSHAN XU, University of Tennessee, Knoxville, MANUEL ANGST, Oak Ridge National Laboratory, TATIANA BRINZARI, University of Tennessee, Knoxville, RAPHAEL HERMANN, Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, Université de Liège, JANICE MUSFELDT, University of Tennessee, Knoxville, ANDY CHRISTIANSON, Oak Ridge National Laboratory, DAVID MANDRUS, Oak Ridge National Laboratory, University of Tennessee, BRIAN SALES, Oak Ridge National Laboratory, STEVE MCGILL, National High Magnetic Field Laboratory, JONG-WOO KIM, Ames Laboratory, ZAHIRUL ISLAM, Argonne National laboratory — We investigated the series of temperature and field-driven transitions in LuFe$_2$O$_4$. Magnetization and x-ray scattering in order to understand the interplay between charge, structure, and magnetism in this multiferroic material. We demonstrate that charge fluctuation has an onset well below the charge ordering transition, supporting the “order by fluctuation” mechanism for the development of charge order superstructure. Bragg splitting and large magneto optical contrast suggest a low temperature monoclinic distortion that can be driven by both temperature and magnetic field.

1 This work is supported by the U.S. Department of Energy.

1:03PM Z30.00010 Electronic approaches on orbital anisotropy and spin configuration in Multiferroic LuFe$_2$O$_4$. K.-T. KO, POSTECH, H.-J. NOH, Chonnam National University, B.-G. PARK, POSTECH, J.-Y. KIM, PAL, J.-H. PARK, POSTECH, A. TANAKA, Hiroshima University, SUNG-BAEK KIM, POSTECH, S.-W. CHEONG, Rutgers University — The orbital anisotropy and spin configuration of the multiferroic LuFe$_2$O$_4$ are investigated by the x-ray absorption spectroscopy (XAS) at Fe $L_3$- and O $K$-edges, and the theoretical cluster model calculations including the configuration interactions and full multiplets. The x-ray magnetic circular dichroism (XMCD) results show that the system has a surprisingly large orbital moment as large as $m_O \sim 0.8 \mu_B/f.u.$, which also agrees with the theoretical calculation result. This result also well explains the observed total magnetic moment of 2.9 $\mu_B/f.u.$ The polarization dependent XAS enables us to identify the orbital level and occupation, which turns out to be rather different from the band structure prediction. We also found that the charge order plays an essential role for the 0.7 eV charge gap. Finally, we discuss the local electronic structure, orbital anisotropy, and the spin configuration of LuFe$_2$O$_4$.

1:15PM Z30.00011 Multiple magnetic transitions and glass dynamics in LuFe$_2$O$_4$. HARI SRIKANTH, MANH-HUONG PHAN, NATALIE FREY, University of South Florida, MANUEL ANGST, BRIAN SALES, DAVID MANDRUS, Oak Ridge National Laboratory — LuFe$_2$O$_4$ is a complex oxide of topical interest as ferroelectricity in this material arises from charge ordering and it also exhibits multiferroic behavior. A good understanding of the magnetic phase diagram has remained elusive due to the complexity of the system as well as the sensitivity to sample quality. In this study, we report on the magnetic properties of high quality LuFe$_2$O$_4$ single crystals grown by the floating zone method. Temperature dependent DC, AC susceptibility and isothermal magnetization reveal a rich and complex phase diagram. Magnetic transitions at 240K and 175K are accompanied by strong frequency dependence of the real ($\chi'$) and imaginary ($\chi''$) parts of the AC susceptibility indicative of glassy behavior. Quantitative fits to the glass model confirm cluster glass dynamics and this is consistent with the presence of ferrimagnetic domains within the Fe-O planes. Magnetocaloric effect (MCE) in these materials will also be presented. We will place our results in the context of work by other groups on this system and clarify the nature of the magnetic phase diagram that emerges from our studies.

1Work supported by DOE.

1:27PM Z30.00012 Stacking the Collinear Magnetic Phases of the Geometrically-Frustrated Antiferromagnet CuFeO$_2$. RANDY FISHERMAN, FENG YE, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory — The correct stacking of hexagonal layers is used to obtain accurate estimates for the exchange and anisotropy parameters of the geometrically-frustrated antiferromagnet CuFeO$_2$. Those parameters are highly constrained by the stability of a collinear metamagnetic phase between fields of 13.5 and 20 T. Constrained fits of the spin-wave frequencies of the “up up down down” phase below 7 T are used to identify the magnetic unit cell of the metamagnetic “up up down down” phase, which contains two hexagonal layers and 10 Fe$^{3+}$ spins. The resulting exchange parameters are much smaller than those obtained from an unconstrained fit of the zero-field spin-wave data and successfully describe not only the main branch of spin-wave excitations but also the spin-wave excitations of the two twins in the $\{H,K,0\}$ plane $^1$. Research sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy under contract with UT-Battelle, LLC. $^1$ R.S. Fishman, F. Ye, J.A. Fernandez-Baca, J.T. Haraldsen, and T. Kimura, Phys. Rev. B 78, 140407 (2008).
Site occupancy and magnetic properties of aluminum substituted barium hexaferrite, AMITAVA MOITRA, SUNGHO KIM, SEONG-GON KIM, Mississippi State University, YANG-KI HONG, University of Alabama, STEVEN C. ERWIN, Naval Research Laboratory — Aluminum substituted barium hexaferrite has been studied using density functional theory (DFT). The substitution has been carried out for BaFe_{12-χ}Al_{χ}O_{19} from χ = 1 to χ = 3 in steps of 0.5. With the aid of accurate DFT study, our result show that the Al^{3+} ions preferentially occupy the 2a and 12k site, unlike the previously reported 4f2, 2a, 4f1, and 12k sites. Our result confirms the experimental fact that with increasing of Al substitution the total magnetic moment monotonically decreases. We also present a possible reason of the site preference of 2a and 12k site, unlike the previously reported 4f2, 2a, 4f1, and 12k sites.

Magnetoelectric Coupling and Relaxation in Yttrium Iron Garnet, YUCHI YAMASAKI, YUKI KOHARA, University of Tokyo, YOSHINORI TOKURA, University of Tokyo, ERATO-JST, and RIKEN — We report the results of the magnetic and dielectric relaxation measurement on yttrium iron garnet Y_{2}Fe_{3}O_{12} which shows the 2nd order magnetoelectric (ME) effect under an applied electric field [1] and the 1st order ME effect by an electric field cooling procedure [2]. We found that the temperature dependence of the dielectric relaxation dynamics coincides with that of magnetic one. This suggests a strong magneto-electric coupling between dielectric and magnetic relaxation dynamics. Indeed the dielectric relaxation strengths are enhanced by an applied magnetic field; namely the amplitude of electric dipole moment can be tuned by magnetic field. This effect accounts for the magnetic field induced change of the static dielectric permittivity and thereby the gigantic 2nd order ME effect as observed. [1] T.H. O’Dell, Phil. Mag. 16, 487 (1967), [2] H. Ogawa et al., JPSJ 56, 452 (1987).

Dielectric and magnetic properties of the Non-centrosymmetric Fe-Lagarosite, NARA LEE, YOUNG JAI CHO, SANG-WOOK CHEONG, Rutgers University — The non-centrosymmetric compound Ba_{2}NbFe_{5}S_{12}O_{19} known as the Fe-lagarsite forms in a unique magnetic triangular lattice of Fe^{3+} spins. The interesting magnetic and dielectric properties may arise from the spin frustration of the triangular magnetic lattice as well as the broken inversion symmetry of the crystallographic structure. In order to understand the complex structure and magnetic spin ordering, we have performed comprehensive experiments on single crystals grown by a floating zone method, including x-ray diffraction analysis and measurements of magnetic susceptibility, dielectric constant and heat capacity under variation of temperature and magnetic field.

Crystal Structure and Magnetic properties of Fe-substituted nanoscale Hydroxypatite, ANDREAS KYRIACOU, RICCARDO VENTURELLI, KOREY SORGE, THEODORA LEVENTOURI, Department of Physics and Center for Biological and Materials Physics, Florida Atlantic University, Boca Raton FL 33431, USA — Magnetic nanoscale hydroxyapatite (HAp) of chemical formula Ca_{1-x-y}Fe_{x}(PO_{4})_{3}OH has been prepared by a chemical precipitation method where x varies from 0 to 1.26. Single phase HAp is identified in XRD patterns of samples with x ≤ 0.30 while maghemite (Fe_{2}O_{3}) is formed as a secondary phase for x ≥ 0.60. The average crystal size as calculated by the Scherrer equation varies from 16 nm to 28 nm. Rietveld refinement reveals a decrease of the unit cell for x ≤ 0.15. Magnetic moment measurements as a function of temperature at applied field μ_{A}H = 1.5 T shows a two component system: a temperature-dependent paramagnet (PM) or superparamagnet (SPM) and a roughly temperature-independent ferromagnetic (FM) component. No FM activity is shown for low x, followed by increased activity for higher x. Increasing SPM activity is observed for x ≥ 0.60. Hysteresis measurements show irreversible loops for x ≥ 0.22.

Structure determination of CoPt nanoparticles: Chemical ordering and its effect on magnetic properties, NILS BLANC, LAUREN BARDOTTI, MATTHIAS HILLENKAMP, ALEXANDRE TAMION, FLORIAN TOURNUS, JULIETTE TUAILLON-COMBES, VERONIQUE DUPUIS, LPMCN, EDGAR BONET, HELIO TOLENTINO, ALINE RAMOS, MAURIZIO DE SANTIS, Institut Neel, PHILIPPE OHRESSER, Synchrotron SOLEIL, THIERRY EPIERCIER, Laboratoire MATEIS — Due to the huge magnetocrystalline anisotropy of bulk CoPt crystallized in the L1_{0} phase, CoPt nanoparticles have been widely studied during the last decade. In order to determine the intrinsic magnetic properties of CoPt clusters, we synthesize benchmark samples: 3 nm diameter CoPt clusters, pre-formed in the gas phase, are embedded in an amorphous carbon matrix under UVH conditions. The transition from the chemically disordered A1 to the ordered L1_{0} phase is then obtained by annealing. Chemical ordering has clearly been evidenced by different techniques (HRTEM, GIXRD). In the case of nanoparticles, this phase transition goes with a magnetic anisotropy increase much lower than for the bulk. Besides, XMCD measurements have revealed a μ_{A}L/μ_{A}S increase for Co and Pt atoms and a strong μ_{A}S enhancement for Co upon L1_{0} ordering. F. Tournus et al. Phys. Rev. B 77, 144411 (2008) Thanks are due to the CLYM (Centre Lyonnais de Microscope) for the access to the transmission electron microscope.

Origin of magnetic anomalies and relaxation mechanisms in ferrofluids, M. B. MORALES, M. H. PHAN, N. A. FREY, S. PAL, H. SRIKANTH, Dept. of Physics, University of South Florida — From a fundamental physics perspective, it is proposed that blocking of magnetic nanoparticles and a carrier of freezing would affect the magnetization and relaxation processes in ferrofluids. To verify this hypothesis, we have conducted systematic DC magnetization and AC susceptibility studies in different ferrofluids composed of Fe_{3}O_{4} and CoFe_{2}O_{4} nanoparticles suspended in hexane and dodecan, which respectively have freezing temperatures below (178K) and above (264K) the blocking temperature of magnetic nanoparticles (~200K). Experimental results reveal that the particle blocking and carrier fluid freezing effects play key roles in the formation of glass-like relaxation peaks in ferrofluids, which remained largely unexplained in previous studies. It is also shown that the nature of these peaks is strongly affected by varying particle size and carrier fluid medium. Quantitative fits of the frequency dependent AC susceptibility to the Vogel-Fulcher model, f = f_{0}exp[E_{a}/(k(T-T_{f})], clearly indicate that the blocking of magnetic nanoparticles in the frozen state significantly affects the interparticle dipole-dipole interaction, causing characteristic spin-glass-like dynamics. A clear correlation between the blocking and freezing temperatures emerges from our studies for the first time.

Competing effect of blocking and spin frustration in nanostructured gadolinium iron garnets, M.H. PHAN, M.B. MORALES, H. SRIKANTH, University of South Florida, C.N. CHINNASAMY, V.G. HARIS, Northeastern University — The ground state magnetic properties and relaxation mechanism in magnetically frustrated system of Gd_{3}Fe_{5}O_{12} is of topical interest due to its complex magnetic structure. As a consequence of geometric and magnetic frustrations, the Gd_{3}Fe_{5}O_{12} system is expected to show glassy magnetic behavior. Through a comprehensive study of DC magnetization, AC susceptibility, transverse susceptibility, and magetocaloric effect in Gd_{3}Fe_{5}O_{12} bulk and nanostructured materials, we provide physical insights into the glassy nature and magnetic relaxation mechanisms in the gadolinium iron garnet system. It is shown that bulk Gd_{3}Fe_{5}O_{12} undergoes two different glassy states at temperatures below its compensation temperature with the low temperature glassy state strongly influenced by Gd ordering. However, the glassy nature is largely suppressed in Gd_{3}Fe_{5}O_{12} nanoparticles in which the blocking phenomenon competes with the spin frustration effect. As particle size is decreased, the blocking effect is dominant over the spin frustration effect. As a result, the nanostructured system shows magnetic relaxation features arising mainly from superparamagnetism.
12:03PM Z31.00005 Thermoinduced Magnetization in NiO Nanoparticles, GREGORY BROWN, Oak Ridge National Laboratory — The low-temperature magnetic susceptibility for model NiO nanoparticles is calculated using the Monte Carlo method, and three different behaviors are seen. With uncompensated spins present, the susceptibility diverges as $T^{-\alpha} \rightarrow 0$. For cube-shaped nanoparticles, a temperature-dependent thermoinduced magnetization is observed. For spherical and octahedral nanoparticles, a temperature-independent susceptibility associated with the spin-flop configuration is observed. Calculations for arbitrary values of the uniaxial anisotropy indicate that thermoinduced magnetization can be observed for all geometries in materials with strong enough anisotropy. This work was supported by the LDRD program of ORNL, by the DOE-OS through the Offices of BES, Division of MSE and ASCR, MICS Division. The V–Mag tool set was developed as part of a BES sponsored Computational Material Science Network project. ORNL is managed by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725.

12:15PM Z31.00006 Magnetic and EPR Characterization of Ni(core)/NiO(shell) Nanoparticles, SARITHA NELLUTLA, ALEX SMIRNOV, JUNWEI WANG, JOSEPH B. TRACY, North Carolina State University — Core/shell nanoparticles have interesting applications in various fields [1-4]. Among these systems, ferromagnet(core)/antiferromagnet(shell) are of particular importance because of their potential use as MRI contrasting agents, high density magnetic recording devices, etc. [3, 4]. Here, Ni(core)/NiO(shell) nanoparticles of different core sizes ranging from 8 nm to 22 nm have been synthesized and characterized by TEM, magnetic susceptibility and electron paramagnetic resonance (EPR) spectroscopy, as "free" (non-agglomerated) particles and agglomerated clusters. Using EPR at 9.1 GHz it is shown that the temperature dependence of the g-value and the EPR linewidth are similar for both the free particles and the agglomerated clusters. This suggests that at this magnetic field (~0.3 T) the EPR signal arises mostly from the saturated magnetic moment. EPR measurements at multiple fields/frequencies provide further insight on the microscopic magnetic structure in the free particles and the agglomeration effects. [1]. M. A. Hines, P. Guyot-Sionnest, J. Phys. Chem., 100, 468 (1996). [2]. Z.C. Xu, Y.L. Hou, S.H. Sun, J. Am. Chem. Soc., 129, 8698 (2007). [3]. V. Skumryev, S. Stoyanov, Z. Zhang, G. Hadjipanayis, D. Givord, J. Nougues, Nature 423, 850 (2003). [4]. A. Hütten, D. Sudfeld, T. Ennen, G. Reiss, W. Hachmann, U. Heinemann, K. Wojczykowski, P. Justzi, W. Saikaly, G. Thomas J. Biotechnology 112, 47-63 (2004).

12:27PM Z31.00007 Development of Novel Biopolymer/Synthetic-Polymer/Iron Oxide Nanocomposites, MARLETH MENA MONTOYA, SUGEHEIDY CARRANZA, MOISÉS HINOJOSA, VIRGILIO GONZÁLEZ, FIME-UANL — In this work we report the successful development of a family of magnetic nanocomposites based on chitosan/or/polyamide 6 matrix with dispersed iron oxide nanoparticles synthesized by chemical co-precipitation. The iron oxide contents varied from 5 up to 23 wt%, the nanocomposites were studied by FTIR, UV-vis, TGA, XRD, TEM and magnetometry. The FTIR analysis demonstrates an interaction between the amide group of the polyamide 6 and the ceramic material. In formic acid, the nanocomposites absorb in the UV-Vis range, and the magnitude of the band gap (optical), calculated using the band of higher wavelength, is between 2.16 and 2.19 eV. In nanocomposites with chitosan/polyamide 6 matrix the developed morphologies are spherulites of polyamide 6 surrounded by chitosan, with the iron oxide particles presumably in the form of ferrititide. The measured magnetic properties revealed a superparamagnetic character on the studied specimens.

12:39PM Z31.00008 Characterization of ultrasonically prepared γ-Fe$_2$O$_3$/Al$_2$O$_3$ shell-core nanocomposites, MATTHEW VANNETTE, JOSHUA HUGEN, DANIEL STOECKLEIN, BRETT MCCARTY, RUSLAN PROZOROV, Ames Lab/Dept. of Physics and Astronomy, Iowa State University — High intensity ultrasonic irradiation (sonication) of slurries of Al$_2$O$_3$ nanopowder in an Fe(CO)$_5$/decane mixture produce superparamagnetic γ-Fe$_2$O$_3$ shells on non-magnetic cores. In this contribution we discuss the effect of the various adjustable parameters (sonication time and intensity, powder loading, and Fe(CO)$_5$/decane ratio) on the dc and ac magnetic properties of these composite materials. Effects of post production modification such as heat treating powders and cold pressing pellets is also presented for a subset of samples.

12:51PM Z31.00009 Phase Transformation in Silica-Coated FePt Nanoparticles, LEVENT COLAK, GEORGE HADJIPANAYIS, University of Delaware — The A1 to L1$_0$ phase transformation has been examined in silica-coated FePt particles. The nanoparticles were synthesized by reduction of platinum acetylacetonate (Pt(acac)$_2$) followed by thermal decomposition of iron pentacarbonyl (Fe(CO)$_5$) in the presence of oleic acid (OA) and oleyl amine (OY) as surfactants at low temperature [1]. The monodispersed FePt nanoparticles, with a size of 5.8 nm were then coated with silica (SiO$_2$) shells [2]. The thickness of the silica shell could be controlled between 7.5-25 nm. The coated particles were subjected to thermal processing at 900 °C for various amounts of times. No significant sintering was observed up to 2 hours of annealing for the shell thickness of 15.0 nm. In some silica-coated samples an increase in the particle size was observed after annealing. Selected Area Diffraction analysis and magnetic measurements showed the development of ordered L1$_0$ structure. Coercivity values up to 15 kOe at 7K are obtained. The phase transformation is currently being examined in other samples annealed at different times and temperatures and the results will be reported.1. Levent Colak and George C. Hadjipanayis, Nanotechnology 19 (2008) 235703.2.M. Aslam, L. Fu, S. Li, Vinayak P. Dravid, Journal of Colloid and Interface Science 290 (2005) 444-449.

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1:03PM Z31.00010 Crystallization thermodynamics and kinetics of SmCo$_5$/Fe system, CHUAN-BONG RONG, J. PING LIU, Department of Physics, University of Texas at Arlington, Arlington, TX 76019 — High energy ball milling is an effective and economic way to produce the hard/soft nanocomposite permanent magnetic materials which have immense potential to exhibit much higher energy products than the conventional single phase hard magnets. Intermetallic materials undertaken high energy ball milling are usually of amorphous structures. It is therefore necessary to study the grain nucleation and growth behavior of the ball-milled amorphous powders. There has not been a systematical study of thermal dynamic and kinetic behavior of the mechanically milled nanocomposite powders. In this work, powder mixtures of SmCo$_5$ + α-Fe (α=0-30 wt%) were mechanically milled for 2 - 10 hours. The thermal dynamic and kinetic behavior of the powders was studied by measuring the differential scanning calorimetry (DSC) curves with different heating rate and isothermal methods. It was observed that the crystallization process of the SmCo$_5$ phase shifted to higher temperature while that of Fe phase shifted to low temperature with increasing milling time. Kissinger analysis shows that the activation energy of SmCo$_5$ phase significantly decreased with increasing milling time and increasing Fe content. Isothermal analysis showed that the nucleation of SmCo$_5$ phase started around 300-350 °C which is 100-150 °C lower than the crystallization temperature (460 °C).

1:15PM Z31.00011 Magneto-structural study of phase pure α and β type MnAs nanoparticles, P. KHAREL, KEERTHI SENEVIRATHNE, RON TACKETT, STEPHANIE BROCK, G. LAVES, Wayne State University — There is extensive interest in understanding the properties of nanoscale materials that exhibit magneto-structural phase transitions because of their possible use in magnetocaloric applications. Bulk MnAs exhibits a ferromagnetic transition in the range 313-317 K, together with a structural transition from a hexagonal (α-MnAs) to an orthorhombic (β-MnAs) lattice. We have studied the structural and magnetic properties of α-MnAs and β-MnAs nanoparticles synthesized using solution-phase arrested precipitation method. XRD and TEM studies show that both the α and β phase nanoparticles are crystalline, phase pure, and stable for weeks at room temperature. Magnetic measurements show that both the α-MnAs and β-MnAs phase nanoparticles undergo ferromagnetic phase transitions near 315K, but we find no evidence for the associated α to β structural transition seen in bulk MnAs. We will present an experimental investigation on the connection between structural and magnetic properties in α and β type MnAs nanoparticles, and discuss relevance to studies on other nanostructured systems.
1:27PM Z31.00012 Magnetic Force Microscopy of Ferromagnetic MnAs Nanoparticles in GaAs.

BEN CHAPRUT, RADIHKAR BARUA, LAURA LEWIS, DON HEIMAN, Northeastern University — The switching behavior and anisotropy of ferromagnetic MnAs nanoparticles in GaAs was investigated with variable-temperature magnetic force microscopy. Nanoparticles of MnAs were synthesized by annealing thin layers of GaMnAs, with Mn/Ga=0.1. Annealing at 640°C resulted in thin disc-shaped MnAs particles with diameters ~100 nm embedded in GaAs. Magnetization measurements at room temperature show that the samples are ferromagnetic and exhibit hysteresis with a coercive field ~0.1 T. In MFM images at room temperature, the majority of the nanoparticles have a single-domain magnetic dipole moment which can be oriented in one direction after applying a magnetic field ~0.1 T. The dipole orientation can be reversed after applying a field in the opposite direction. After raising the temperature above the Curie point, Tc=337 K, the sample becomes demagnetized at room temperature, with equal numbers of particles aligned in opposite directions. A sharp phase transition, from the ferromagnetic hexagonal phase to the paramagnetic orthorhombic phase, was found at 340°C, nearly coincident with the Curie temperature. This transition occurs ~30°C higher than in thin MnAs films and is attributed to tensile strain on the nanoparticles from the surrounding GaAs.

1:39PM Z31.00013 Nanoparticulate Alnico Thin Films with High Coercivity1.

OZAN AKDOGAN, GEORGE C. HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Newark, DE, U.S.A. — Alnico V (Fe-8% Al-14% Ni-24% Co-3% Cu) nanoparticulate thin films have been produced by dc magnetron sputtering. The films were sputtered on Si substrates for magnetic measurements and carbon-coated copper grids for TEM measurements. The as-deposited films have a fine-grained microstructure with the bcc crystal structure. The as-made films were subjected to a full heat treatment which consists of heating the sample to 900°C, then cooling it to 600°C and finally annealing it at 600°C for several hours. After the heat treatment, the thin films broke up into large nanoparticles (20-60 nm) surrounded by small nanoparticles (2 nm). Electron diffraction data showed that the annealed samples had an fcc structure. The maximum room temperature coercivity was found to be 2 kOe after 6h of annealing at 600°C. The high coercivity could be due to strain that was induced during precipitation. The evolution of crystal structure and microstructure with annealing will be monitored and related to the observed magnetic properties.

1Work supported by NSF DMR-0302544.

1:51PM Z31.00014 Magnetic Properties of As-Prepared and Annealed Nanocrystalline Fe Particles.

KARL UNRUH, THOMAS EKIERT, University of Delaware — Air stable Fe-core/oxide-shell particles with diameters between about 100 and 200 nm have been synthesized by the reduction of a ferrous Fe salt in the presence of citrate ions. Structural, chemical, and magnetic measurements indicate that the oxide shell is 2-3 nm thick and that the core consists of essentially oxide free, α-Fe nanocrystals (about 5 nm in diameter) in addition to regions of non-crystalline, disordered Fe. The as-prepared particles evolve into a continuous porous solid structured at about the 100 nm scale after annealing in forming gas at temperatures near 750°C followed by a progressive elimination of the porosity at higher annealing temperatures. Prior to the formation of the porous solid the saturation magnetization, coercivity, and remanence ratio all increase slightly with annealing temperature due to an increase in the size of the core Fe crystallites at the expense of the disordered Fe component. The structural transformation to a porous solid, however, results in an abrupt increase in both the coercivity (by about 50% at 300 K and 100% at 5 K) and remanence ratio (about 100% at 300 K and 150% at 5 K).

2:03PM Z31.00015 Anisotropic Sm-Co(Fe) Nanoparticles Produced by Surfactant-Assisted Ball Milling1.

NILAY GUNDUZ-ASKDOGAN, GEORGE C. HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Newark, DE, U.S.A., DAVID J. SELLMYER, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588 USA. — Magnetic hard SmCo and Sm2(Co8-δFe2δ)-17 nanoparticles have been produced by using surfactant assisted low- and high-energy ball milling. Surfactants prevent the re-welding of the crashed nanoparticles during the milling process and thus limit the particle growth. Oleic acid was used as the surfactant and the heptane as the milling medium. High energy ball milling experiments took place in a milling vial with carbon steel balls by using a Spex 8000M high energy ball milling machine. The coercivity was found to increase with milling time with a value of 2.9 kOe for Sm2(Co8.5Fe2.5)17 and 19.5 kOe for SmCo5 after 12 hrs of milling. TEM data showed that the milled powders have a narrow size distribution. The TEM grid-deposited samples showed self-assembled nanoparticles in the Sm2(Co8-δFe2δ)17 alloy after 4 hours of milling, which could be further aligned when subjected to a magnetic field. The evolution of structural and microstructural properties of the particles will be monitored and compared with their magnetic properties.

1Work supported by DOE DE-FG02-04ER4612.

Friday, March 20, 2009 11:15AM - 1:51PM —
Session Z32 GMAG DMP FIAP: Focus Session: Magnetoresistance and Spin-dependent Transport

11:15AM Z32.00001 Nitrogen doping in single-crystal MgO magnetic tunnel junctions.

JUSTIN BROCKMAN, CHENG-HAN YANG, IBM / Stanford, MAHESH SAMANT, KEVIN ROCHE, STUART PANKIN, IBM — Recent experiments have shown evidence for induced ferromagnetism in thin films of carbon and nitrogen-doped zinc oxide. We have discovered similar behavior in nitrogen-doped MgO films grown by plasma-assisted thermal evaporation. Here, we incorporate these films as tunneling barriers into single-crystal multilayer magnetic tunnel junctions and present experimental results showing the magnetoresistance and current-voltage characteristics for these structures.

11:27AM Z32.00002 Bias dependence of Fe-MgO-Fe magnetic tunnel junction devices within a single-band tight-binding model.

TEHSEEN RAZA, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, HASSAN RAZA, School of Electrical and Computer Engineering, Cornell University, Ithaca NY. 14853 — We have developed a transferable single-band tight-binding model benchmarked with the ab initio methods for Fe-MgO-Fe magnetic tunnel junction (MTJ) devices [1]. The computational complexity of our model is on the order of an effective mass one, but additionally it includes the bandstructure physics over the two-dimensional transverse Brillouin zone in an average manner. We study the bias dependence of the tunnel magnetoresistance (TMR) ratio in MTJ devices. At low bias, for both the 4-layer and 12-layer MgO barrier, the TMR is bias-independent. It is higher for the 12-layer device due to relatively a larger decrease in the AP current density. At high bias, our model predicts a sharp roll-off in TMR ratio, which is attributed to a rapid increase in the Delta1 band current density in the anti parallel (AP) configuration due to the bandedge states entering the conduction window. The TMR ultimately becomes negative when the AP current becomes higher than the P current due to the different k-states tunneling through the same barrier. [1] T. Z. Raza and H. Raza, arXiv:0804.2957
11:39 AM Z32.00003 Magnetoresistance in Double Spin Filter Tunnel Junctions with Nonmagnetic Electrodes and Its Unconventional Bias Dependence1, GUO-XING MIAO, MARTINA MULLER, JAGADEESH MOODERA, MIT — We demonstrate a large tunnel magnetoresistance (TMR) originating purely from the tuning of tunnel barrier heights in double barrier junctions with nonmagnetic electrodes. This is achieved by the spin filtering that occurs due to the selective tunneling probabilities for spin-up and -down electrons through a magnetic semiconductor barrier resulting in highly spin polarized tunnel currents. Combining two such barriers in a tunnel junction thus leads to a TMR without the necessity of magnetic electrodes. This is significantly different from traditional approaches for generating TMR involving two ferromagnetic electrodes and for example, using Al2O3 or MgO barriers. We demonstrate the first realization of such unconventional tunnel junctions and TMR using EuS / EuO based spin filter barriers with nonmagnetic Al electrodes. The novel non-monotonic and asymmetric bias behavior in magnetoresistance can be qualitatively modeled in the framework of WKB approximations.

1Work supported by NSF, ONR and KIST-MIT project funds.

11:51 AM Z32.00004 The critical role of the barrier thickness in spin filter tunneling1, CASEY MILLER, University of South Florida, Department of Physics — Spin filter tunneling is considered in the low bias limit as functions of the temperature dependent barrier parameters. We demonstrate the generation of spin polarized tunneling currents in relation to the magnetic order parameter, and discuss how an interfacially suppressed order parameter leads to a temperature dependent tunneling current asymmetry. Analyzing the full parameter space reveals that the often overlooked barrier thickness plays a critical role in spin filter tunneling. With all else fixed, thicker barriers yield higher spin polarization, and allow a given polarization to be achieved at higher temperatures.

1Supported by NSF Award No. ECCS-0820880

12:03PM Z32.00005 Spin-Dependent Electronic Transport in Fe/MnAs/Fe Structures, KYUNG-YEON KIM, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We have performed first-principles calculations of electronic structures and tunnel magnetoresistances of Fe/MnAs/Fe structures, which are junctions of two semi-infinite metals and a half-metal placed between them. The electronic structures are described by the Kohn-Sham density functional theory, with local spin density approximation, norm-conserving semicore pseudopotentials, and pseudo-atomic orbital basis set. The tunnel magnetoresistance is obtained by using a scattering- state method, considering different configurations of the magnetization. This work was supported by the KRF (KRF-2007-314-C00075) and by the KOSEF Grant No. R01-2007-000-20922-0. Computational resources have been provided by KISTI Supercomputing Center (KSC-2008-S02-0004).

12:15PM Z32.00006 Spin dependent transport in FeCo|MgBO|FeCo magnetic tunnel junctions: Can boron in the oxide region be a good thing?, DEREK STEWART, Cornell Nanoscale Facility, Cornell University — Recent experimental studies on FeCoB/MgO/FeCoB tunnel junctions have shown that boron can diffuse into the oxide region during rf-sputtering and result in the formation of crystalline MgBO regions[1,2]. These tunnel junctions still provide high tunneling magnetoresistance values as well as very low RA products[3]. Using a plane wave-pseudopotential density functional approach, I have examined potential Mg(B) oxides such as MgB2O4 as well as kotoite (Mg2B2O5). Total energy calculations indicate that these oxides should be more stable than the formation of separate regions of MgO and B2O3. Kotoite (Mg2B2O5) also has a boron concentration close to that found in the experimentally grown MgBO regions. In addition, kotoite provides a good lattice match with MgO and could act to template neighboring FeCo into crystalline bcc layers during annealing. This evidence suggests that kotoite is formed during the deposition process. I will also discuss the complex band structure of kotoite (Mg2B2O5) and examine how this will also affect spin dependent transport from the FeCo leads. [1] J. Y. Bae et al., J. Appl. Phys. 99 08T316 (2006) [2] J. C. Read et al., Appl. Phys. Lett. 90 132503 (2007) [3] J. C. Read personal communication

12:27PM Z32.00007 Effect of thermal spin disorder on transport through magnetic tunnel junctions, ALEKSANDER WYSOCKI, KIRILL BELASCHENKO, Department of Physics and Astronomy, University of Nebraska Lincoln — We study the transport properties of Fe1−xMgOFe1−xMgO tunnel junctions in the presence of spin disorder using the noncollinear density functional theory. For a given temperature the spin disorder in ferromagnetic leads is introduced by randomizing the directions of spin densities in atomic spheres according to the mean-field angular distribution function. For pure FeMgOFe we found that even small spin disorder has a dramatic effect on transmission as compared to the zero temperature case due to the presence of interface states in the minority spin channel that are strongly affected by spin disorder. This results in a complicated temperature dependence of the tunneling magnetoresistance (TMR). On the other hand, in the case of Fe1−xMgOFe1−xMgO the interface states are less important and the main effect of the spin disorder is to decrease the spin polarization diminishing TMR. The temperature dependence of TMR is in agreement with Julliere model prediction with the spin polarization being proportional to magnetization.

12:39PM Z32.00008 Evolution of low-frequency resistance noise during annealing in CoFeB/MgO/CoFeB tunnel junctions1, RYAN STEARRETT, WEIGANG WANG, LUBNA SHAH, EDMUND NOWAK, JOHN XIAO, University of Delaware — We have studied the evolution of tunneling magnetoresistance (TMR) and resistance noise in magnetic tunnel junctions (MTJs) as a function of annealing time at 425°C. Previously, we showed that short annealing times do lead to significant improvement in the MgO crystal structure and crystallization of the CoFeB electrodes, resulting in large TMR values up to 200%. We also observe that the low-frequency resistance noise decreases significantly after annealing for only a few minutes. The resistance noise has a 1/f spectrum and is quantified by a Hooge-like parameter, α, given in units of μm². In unannealed samples α is of order 10⁻⁹ μm² and decreases with increasing voltage bias. Upon annealing, α drops to 10⁻¹⁰ μm² and is less dependent on bias, particularly in the parallel configuration. We attribute the decrease in α and its bias dependence, α(V), to a reduction of defects in and around the barrier due to annealing. The implications for optimizing the signal to noise ratio of MgO-based MTJ sensors will also be discussed.

1Department of Energy

12:51PM Z32.00009 ABSTRACT WITHDRAWN —
1:03PM Z32.00010 Current-Perpendicular-to-Plane Magnetoresistance of CoFe-based Exchange-Biased Spin-Valves1. CHIYUI AHN, KYUNG-HO SHIN, Korea Institute of Science and Technology, REZA LOLLOEE, JACK BASS, WILLIAM PRATT, Michigan State University — Concentrated Co(50)/Fe(50) and Co(70)/Fe(30) alloys are of interest for spintronics applications. We have constrained the spin-transport properties of these alloys by measuring at 4.2 K the specific resistance (CPP area times resistance) and magnetoresistance of exchange-biased spin-valves (EBSVs) of the form (FeMn/CoFe/Cu/CoFe)—here CoFe indicates one of the two alloys of interest—where the magnetization of one CoFe layer is exchange bias pinned by the adjacent antiferromagnetic FeMn layer, and the magnetization of the other CoFe layer is free to switch from parallel (P) to anti-parallel (AP) to that of the pinned layer in a modest magnetic field. For each CoFe alloy, we have measured EBSVs where the thicknesses of both the fixed and free layers were held equal and varied together, and EBSVs where the thickness of the pinned CoFe layer was held fixed and that of the free layer was varied. From such measurements we have estimated two parameters: the bulk scattering asymmetry and the spin-diffusion length, for each of the two CoFe alloys. We will present both our data and the derived parameters.

1Work supported by US National Science Foundation grant DMR-0804126 and Korea Institute of Science and Technology.

1:15PM Z32.00011 Specific Resistance of Pd/Ir Interfaces1. RAKHI ACHARYYA, HOANG YEN THI NGUYEN, REZA LOLLOEE, WILLIAM P. PRATT JR., JACK BASS, Michigan State University, SHUAI WANG, KE XIA, Chinese Academy of Sciences — In electronic transport with current-flow perpendicular to the layer planes (CPP) of a metallic multilayer, the interface specific resistance AR (area A through which CPP-

1Supported by US-NSF DMR-08-04126 and China NSF & MOST (No. 2006CB933000).

1:27PM Z32.00012 Enhancement of Biquadratic Coupling in Co/Fe/MgO/Fe(001). JARED WONG, YUEH-FENG CHIANG, ANDREW HOFF, XIAOJING TAN, YAN LI, KEYU PI, WEI HAU WANG, HARRY TOM, ROLAND KAWAKAMI, University of California, Riverside — One interesting aspect of the interlayer exchange coupling (IEC) across MgO is that in addition to the bilinear coupling, a biquadratic coupling favoring 90° magnetization alignment has been observed [1, 2, 3]. We investigate IEC in Co/Fe/MgO/Fe(001) and the affects of non-ideal aspects of the MgO-heterostructure, such as interface oxidation and impurities in the MgO, via molecular beam epitaxy (MBE) synthesis and magneto-optic Kerr effect (MOKE) measurements across aged samples. By independently varying the oxygen content of the MgO film and the Fe/MgO interface, we find that the biquadratic coupling is correlated to the interfacial oxidation. Furthermore, the temperature dependence of the biquadratic coupling exhibits a strong increase at low temperatures. Our findings strongly support the loose spin mechanism as the origin of the biquadratic coupling across MgO[4]. 1. J. Jaure-Vincent, C. Tiusan, C. Bellouard, et al., Phys. Rev. Lett. 89, 107206 (2002). 2. T. Katayama, S. Yuasa, J. Velev, et al., Appl. Phys. Lett. 89, 112503 (2006). 3. E. Snoek, P. Bailes, G. BenAssayag, et al., J. Phys.: Cond. Mat. 20, 055219 (2008). 4. J. C. Slonczewski, J. Appl. Phys. 73, 5957 (1993).

1:39PM Z32.00013 Magnetic tunnel junctions with a ferroelectric barrier using epitaxial La$_{0.7}$Ca$_{0.3}$MnO$_3$/(Ba, Sr)TiO$_3$/La$_{0.7}$Ca$_{0.3}$MnO$_3$ trilayers1. SHENMING GUO, KE CHEN, XIAOXING XI, QI LI, Pennsylvania State University, YONGGANG ZHAO, Tsinghua University — We have fabricated multiferroic tunnel junctions using ferromagnetic La$_{0.7}$Ca$_{0.3}$MnO$_3$ as electrodes and ferroelectric (Ba, Sr)TiO$_3$ as the barrier. We have observed tunneling magnetoresistance as in a typical magnetic tunnel junction (MTJ). Since the ferroelectric barrier can be charge polarized in two opposite directions which alters tunneling conductance, we have observed large tunnelling resistances (~50%) when the charge polarization is switched. This is consistent with the results of both magnetic parallel and antiparallel states. As a result, this type of junctions has four resistance states instead of two for a normal MTJ, corresponding to positive- and negative-polarized parallel and antiparallel states. The four states can be manipulated by the magnetic and electric fields. The dependence of the magnetoresistance and electroresistance as functions of magnetic field, electric field, and bias voltage will be presented.

1This work is supported by NSF.

Friday, March 20, 2009 11:15AM - 2:03PM — Session Z33 DCMP: Fluctuation Phenomena 403

11:15AM Z33.00001 Fluctuations of the superconducting order parameter as an origin of the Nernst effect. KAREN MICHAELI, Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, ALEXANDER FINKELSTEIN, The Weizmann Institute of Science, Israel and Department of Physics, Texas A&M University, College Station, TX 77843-4242, USA — We show that the strong Nernst signal observed recently in amorphous superconducting films far above the critical temperature is caused by the fluctuations of the superconducting order parameter. We demonstrate a striking agreement between our theoretical calculations and the experimental data at various temperatures and magnetic fields. Besides, the Nernst effect is interesting not only in the context of superconductivity. We discuss some subtle issues in the theoretical study of thermal phenomena that we have encountered while calculating the Nernst coefficient. In particular, we explain how the Nernst theorem (the third law of thermodynamics) imposes a strict constrain on the magnitude of the Nernst effect.

11:27AM Z33.00002 Interstate switching induced by non-Gaussian noise1. LORA BILLINGS, Montclair State University, MARK DYKMAN, Michigan State University, IRA SCHWARTZ, US Naval Research Laboratory — We consider the rate of switching between stable states of a dynamical system driven by a non-Gaussian noise. The problem of the switching barrier is reduced to a variational problem of finding a mechanical action for an auxiliary noise-free system. The emphasis of our analysis is placed on the generic system-independent features of fluctuations induced by Poisson noise. If the system is overdamped, Poisson noise leads to switching only for a certain polarity of pulses. This is qualitatively different from the noise effect on underdamped systems. We study the transition between these types of behavior with varying damping. For systems close to a bifurcation point, the barrier height displays a scaling dependence on the control parameter and on the noise parameters. We study parametric dependence for generic types of bifurcations, such as saddle-node and pitchfork bifurcations. Analytical results are compared with the results of detailed numerical simulations.

1Supported by ARO Grant No. W911NF-06-1-0320.
Josephson current noise above $T_c$ in superconducting tunnel junctions

Josephson current noise above $T_c$ in superconducting tunnel junctions

Benjamin Phillabaum, Purdue University, and Yen Lee Lo, Ohio State University

We propose that hysteretic effects in superconducting tunnel junctions may be used as a probe of electronic nematic order in cuprate superconductors. Stripes, a unidirectional, nanoscale modulation of electronic charge, are strongly affected by quenched disorder in two-dimensional and quasi-two-dimensional systems. While stripe orientations tend to lock to ma jor lattice directions, dopant disorder locally breaks rotational symmetry. In a host crystal with otherwise C4 rotational symmetry, stripe orientations in the presence of quenched disorder map to the random field Ising model. We use simulations of the random field Ising model to generate ensembles of local stripe orientations, and then further simulate the effects of such a pattern on the superfluid density within the XY model. We find clear hysteretic effects in the superfluid density anisotropy as a function of applied orienting field.

The authors acknowledge support from Research Corporation and NSF DMR-0804748.

Current-driven quantum switch

M.V. Milosevic, Departement Fysica, Universiteit Antwerpen, Belgium, A. Kanda, S. Hatsumi Hatsumi, Institute of Physics and TIMS, University of Tsukuba, Japan, and F.M. Peeters, Departement Fysica, Universiteit Antwerpen, Belgium, Y. Ootuka, Institute of Physics and TIMS, University of Tsukuba, Japan

We investigate the effect of static anti-phase stripe order on the weak-field Hall effect in superconducting $T_c$ in bi- and trilayers. These interfaces are partially oriented within the crystallographic ab-plane are achieved by tilted epitaxial growth on SrTiO$_3$ (305) substrates. Sharp magnetization switching behavior is observed in the (305) oriented structures, due to the uniaxial magnetic anisotropy. At temperatures close to $T_c$, resistance jumps are induced by magnetization switching. Our results indicate that the switching behavior arises from magnetic stray fields from the ferromagnetic layers that penetrate into the superconductor, rather than spin-switch or spin-accumulation effects.

Theory of Low-Temperature Hall Effect in Stripe-Ordered Cuprates

Jie Lin, Andrew Millis, Department of Physics, and Philip Phillips, University of Illinois at Urbana-Champaign

We investigate the effect of static anti-phase stripe order on the weak-field Hall effect of electrons with dispersion appropriate to the high $T_c$ cuprates. We first consider the cases where the magnitudes of the spin and charge stripe potentials are smaller than or of the same order as the bandwidth of electrons. In a model with only spin stripe potential, and at carrier concentrations appropriate to hole-doped cuprates, the calculated $R_H$ shows sign change as increasing the stripe potential, in semi-quantitative agreement with data. In a charge-stripe-potential-only model, $R_H$ increases as the charge stripe potential increases, with no sign change occurring. In a model with both stripe potentials, $R_H$ may be enhanced or may change sign. We also consider the case in which the magnitudes of the stripe potentials are much larger than the bandwidth, where analytical results can be obtained.

Emergence of Particle-Hole Symmetry near Optimal Doping in High-Temperature Copper Oxide Superconductors

Shiladitya Chakraborty, University of Illinois at Urbana-Champaign

High-temperature copper oxide superconductors (cuprates) display unconventional physics when they are lightly doped whereas the standard theory of metals prevails in the opposite regime. For example, the thermoelectric power changes sign abruptly near optimal doping in a wide class of cuprates, a stark departure from the standard theory of metals in which the thermopower vanishes only when one electron exists per site. We show that this effect arises from proximity to a state in which particle-hole symmetry is dynamically generated. The operative mechanism is dynamical spectral weight transfer from states that lie at least 2eV away from the chemical potential. The emergence of this symmetry close to optimal doping points to pairing in the cuprates being driven by high-energy electronic states.

Exact two-band model of Cu-O planes with charge stripes and plaquettes

Stellan Ostlund, Mats Granath, Gothenburg University

A standard model of the Cu-O planes of high $T_c$ superconductors suggests the relevance of a three-band model of electrons with strong Coulomb repulsion. Particularly dominant is the copper site interaction and charge fluctuations are most strongly suppressed on these sites. We simplify this model further by completely suppressing the charge fluctuations on the copper sites and replacing the copper spins by a spin texture that couples to the local hopping. The resulting generic two-band model of electrons in is then studied for various spin textures on the copper atoms. For general values of the effective hopping parameters, the low energy eigenstates strongly favor charge stripe and plaquette ordering, with a complex multiply connected Fermi surface with the possibility of both pockets and open orbits coexisting. Particularly striking is the emergence of multiparticle ground states that are both delocalized and still effectively minimize nearest neighbor density correlations.

Two-order-parameter theory of magnetism and superconductivity

Victor Galitski, Tudor Stanescu, University of Maryland

Starting with a microscopic interacting electron Hamiltonian, we derive a self-consistent two-order-parameter theory to describe a general case of competing or co-existing magnetic and superconducting instabilities. This is achieved by splitting the initial interaction in two different channels and weighting each channel with an auxiliary field with a non-linear constraint. The double Hubbard-Stratonovich transform leads to a model similar to that in gauge theories. We analyze the resulting theory and argue that generally the magnetic and superconducting fluctuations are equally important and should be treated on equal footing. We discuss the general criteria of the two transitions occurring at similar energy scales and discuss the relevance of these results to superconductivity in the heavy fermion compounds and possibly the cuprates.
11:15AM Z35.00011 Two band model for the cuprates. SHU LIU, STEVEN WHITE, UC, Irvine — We use a numerical canonical transformation approach to derive an effective two-band model for the hole-doped cuprates, which keeps both oxygen and copper orbitals but removes double occupancy from each. A similar model was considered previously by Frenkel, Gooding, Shraiman, and Siggia (PRB 41, number 1, page 350). We compare the numerically derived model with previously obtained analytical results. In addition to the usual hopping terms between oxygens $t_{pp}$ and Cu-Cu exchange terms $J_{cu}$, the model also includes a strong copper-oxygen exchange interaction $J_{po}$ and a Kondo-like spin-flip oxygen-oxygen hopping term $K_{po}$. We use the density matrix renormalization group to study the charge, spin, and pairing properties of the derived model on ladder systems.

11:27PM Z33.00012 Classification of topological insulators and superconductors in three spatial dimensions. SHINSEI RYU, Department of Physics, University of California, Berkeley, ANDREAS SCHNYDER, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, AKIRA FURUSAKI, RIKEN, ANDREAS LUDWIG, Department of Physics, University of California, Santa Barbara — We systematically study topological phases of insulators and superconductors (or superfluids) in 3D. We find that there exist 3D topologically non-trivial insulators or superconductors in five out of ten symmetry classes introduced in seminal work by Altland and Zirnbauer within the context of random matrix theory, more than a decade ago. One of these is the recently introduced $Z_2$ topological insulator in the symplectic (or spin-orbit) symmetry class. We show there exist precisely four more topological insulators. For these systems, all of which are time-reversal invariant in 3D, the space of insulating ground states satisfying certain discrete symmetry properties is partitioned into topological sectors that are separated by quantum phase transitions. Three of the above five topologically non-trivial phases can be realized as time-reversal invariant superconductors, and in these the different topological sectors are characterized by an integer winding number defined in momentum space. When such 3D topological insulators are terminated by a 2D surface, they support stable surface Dirac (Majorana) fermion modes.

11:39PM Z33.00013 Spin-Orbit Scattering and Quantum Metallicity in Ultra-Thin Be Films. PHILIP ADAMS, YIMIN XIONG, AMAR KARKI, DAVID YOUNG, Louisiana State University — We compare and contrast the low temperature magnetotransport properties of ultra-thin, insulating, Be films with and without spin-orbit scattering (SOS). Beryllium films have very little intrinsic SOS, but by “dusting” them with sub-monolayer coverages of Au, one can introduce a well controlled SOS rate. Pure Be films with sheet resistance $R > R_Q$ exhibit a low-temperature negative magnetoresistance (MR) that saturates to the quantum resistance $R_Q = h/e^2$. This high-field quantum metal phase is believed to represent a new ground state of the system. In contrast, the corresponding negative MR in Be/Au films is greatly diminished, suggesting that, in the presence of strong SOS, the quantum metal phase can only be reached at field scales well beyond those typically available in a low temperature laboratory.

11:51PM Z33.00014 Quantum critical point and van Hove singularity in La$_{2-x-y}$Sr$_x$Nd$_y$CuO$_4$. BEN MALLETT, Victoria University, JEFFERY TALLON, Industrial Research Ltd — By means of Zn substitution, thermopower and magnetic measurements we locate, distinguish and track the evolution of the pseudogap critical point and the van Hove singularity as a function of Nd content and relate these to pressure dependent effects in the Nd-free compound. The results have generic implications for all HTS cuprates.

Supported by the Marsden Fund of New Zealand.


11:15AM Z35.00001 Properties of iron selenide single crystals. CEDOMIR PETROVIC, Brookhaven National Laboratory, RONGWEI HU, Brookhaven National Laboratory and Brown University, BROOKHAVEN NATIONAL LABORATORY TEAM — Single crystals of FeSe$_x$ were grown by molten metallic flux technique. Synchrotron powder X-ray diffraction confirms phase purity. Thermodynamic, magnetic and electrical transport properties will be presented.

Supported by the Office of Basic Energy Sciences US Department of Energy

11:27AM Z35.00002 Single crystal growth and anisotropy of magnetic and transport properties of FeTe and FeTe$_{1-x}$Sn$_x$ superconductors. RONGWEI HU, Physics Department, Brown University, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory — Single crystals of FeTe and FeTe$_{1-x}$Sn$_x$ were grown by molten metallic flux technique. Synchrotron powder X-ray diffraction confirms phase purity. We will present anisotropy of magnetic and electrical transport properties in normal and superconducting state of these compounds.

11:39AM Z33.00003 New Fe-based superconductor $S$ doped FeTe using nontoxic elements. YOSHIHIKO TAKANO, YOSHIKAZU MIZUGUCHI, National Institute for Materials Science (NIMS) — Discovery of Fe-based new superconductor was received with considerable surprise. The Fe based-superconductor is expected to be a new series of high-Tc superconductors such as cuprate High-Tcs. However, one of the demerits of Fe based-superconductor is that it contains toxic element of As or Se. So, new Fe based- superconductors composed of nontoxic elements were required. Recently, we have discovered $S$ doped FeTe as a new superconductor using nontoxic elements. Its superconducting transition temperature is around 10K and the upper critical fields is 70T. This material has merit for superconducting applications.

11:51AM Z35.00004 Superconducting and magnetic properties of Fe-Se-Te compounds. C.V. TOMY, G. BALAKRISHNAN, M.R. LEES, Department of Physics, University of Warwick, Coventry CV4 7AL, UK — The discovery of a new Fe based superconductor $a$Fe$_x$Se$_y$ with a $T_c$ of 8 K, hot on the heels of the discovery of superconductivity in LaOFeP/As compounds, has triggered a fresh interest in the study of Fe based superconductors. $S$ can be replaced with Te in FeSe$_{1-x}$Te$_x$, and this results in an increase in $T_c$ from 8 K for $x = 0$ to 15 K for $x = 0.5$ while compounds for $x > 0.8$ are no longer superconducting. We report the synthesis and characterization of the compounds FeSe$_{1-x}$Te$_x$ covering the entire solid solution range. The superconducting transition in resistivity measurements does not show any broadening in magnetic fields up to 9 T, but shifts to lower temperatures linearly with a value $\sim -0.22$ K/T. This results in extremely high upper critical fields ($H_{c2}$) of the order of 70-80 T in these compounds. The superconducting properties are also sensitive to applied pressure and exhibit a positive $dT_c/dP$ of around 0.41 K/kbar for the $x = 0.5$ composition. We observe a jump in specific heat at $T_c$ corresponding to a superconducting gap of 1.8 meV, indicating the bulk nature of superconductivity. Detailed investigations through magnetization, transport and specific heat measurements are presented. A study of the magnetic properties of the non superconducting end compound, FeTe is also presented to gain insight into the onset of superconductivity in the doped systems.

This work supported by DOE under grant Grant DE-FG02-07ER46420.
12:03PM Z35.00005 High Pressure Structure and Transport Properties of the FeSe_{0.88} Superconductor, T. WU, Z. CHEN, T.A. TYSON, Z. QIN, T. ZHOU, Physics Department, New Jersey Institute of Technology, C. ZHANG, S.-W. CHEONG, Department of Physics and Astronomy, Rutgers University — The structure of FeSe_{0.88} was measured for pressures up to 7 GPa using diamond anvil cells in order to probe the changes in the lattice which coincide with change in the transport properties. These measurements are being complemented by high pressure transport measurement over the same pressure range. The trends in structure and transport with pressure will be presented in order to understand the origin of the strong pressure dependence of the superconducting transition temperature.

12:15PM Z35.00006 Superconductivity and antiferromagnetism in Fe(Se_{1-x}Te_{x})_{0.82}, E.K. VEHESTEDT, M.H. FANG, B. QIAN, T.J. LIU, Tulane University, L. SPINU, H.M. PHAM, University of New Orleans, W. BAO, M.R. FITZSIMMONS, M. ZHERNENKOY, Los Alamos, Y. QIU, Q. HUANG, M.A. GREEN, P. ZAJDEL, NIST, J. YANG, Zhejiang University, Y. LIU, Pennsylvania State University, Z.Q. MAO, Tulane University — The search for unconventional superconductors has been reenergized by the discovery of Tc up to 56 K in FeAs type materials [1]. Revelation of the binary superconductor FeSe, Tc = 8 K [2], prompted our investigation of the phase diagram and the evolution of superconductivity and magnetism in the ternary Fe(Se_{1-x}Te_{x})_{0.82} (0 < x < 1.0) system. We discovered a new superconducting phase with Tc,max = 14 K for 0.3 < x < 1.0. End member FeTe_{0.82} is non-superconducting and exhibits incommensurate antiferromagnetic (AFM) order. The AFM order contains both linear and spiral components, propagating diagonally in the Fe tetragonal lattice, in contrast with the commensurate AFM order in FeAs-based superconductors. Superconductivity occurs when the long-range AFM order evolves into short-range correlations with the isovalent substitution of Se for Te. These findings strongly suggest that superconductivity in this system is associated with magnetic correlations, and thus may be unconventional in nature.


12:27PM Z35.00007 ABSTRACT WITHDRAWN

12:39PM Z35.00008 Growth and superconductivity of FeSe_{x} crystals, ZHI LI XIAO*, UMESH PATEL*, SUHONG YU*, HELMUT CLAUS, VITALI VLASTKO-VLASOV, SEVDA AVCI*, JOHN SCHLIEUTER, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory, *Northern Illinois University — Stimulated by the recent discovery of high temperature superconductivity in ferrous pnictides, other iron-based planar compounds have been revisited to search for superconductivity. The most promising outcome of this effort is the discovery of superconductivity in alpha - FeSe which is less toxic but has a FeSe_{x} tetrahedral planar crystal sublattice similar to that consisting FeAs_{x} in the oxypnictides. Investigations on the superconducting in FeSe_{x} can shed light on the superconducting mechanism in oxypnictides. We report the growth of FeSe_{x} crystals through a vapor self-transport approach. Both tetragonal and hexagonal shaped FeSe_{x} crystals with a lateral dimension of up to a few millimeters were obtained and their superconductivity was investigated with both magnetization and resistive measurements. We systematically explored the effect of synthesis parameters such as Fe/Se ratio, sintering temperature and cooling rate on the quality of the crystals.

1 This work is supported by DOE, under contract DE-AC02-06CH11357, Award DE-FG02-06ER46334, and by NSF Grant No. DMR-0605748.

12:51PM Z35.00009 Superconductivity and Antiferromagnetism In Fe(Se_{1-x}S_{x}) System, T.J. LIU, Tulane University, M.H. FANG, B. QIAN, E.K. VEHESTEDT, Tulane University, J.H. YANG, Zhejiang University, H.M. PHAM, L. SPINU, University of New Orleans, Z.Q. MAO, Tulane University — The surprising discovery of superconductivity up to 56 K [1] in FeAs based compounds has reinvigorated the search for unusual superconductors. The recently revealed FeSe superconductor [2] has inspired the community to take a second look at other previously studied materials, such as FeTe. We have investigated properties of Fe(Se_{1-x}S_{x}). Our results show that the solid solution of S in this system is limited, < 30%. We observed superconductivity at 9 K in both polycrystalline samples Fe(Se_{1-x}S_{x}) with 0 < x < 0.3 and 0.86 ≤ y ≤ 1.1, and single crystals with the composition Fe(Se_{0.9}S_{0.1})_91. In addition, our results suggest that this superconducting phase coexists with antiferromagnetism and that the superconducting volume fraction depends on excess Fe at interstitial sites, and excess Fe suppresses superconductivity. This allows us a unique view into the important role of magnetic correlations in mediating superconducting pairing.


1:03PM Z35.00010 Superconductivity of Iron Selenide Thin Films, YUEFENG NIE, ERIND BRAHIMI, JOSEPH BUDNICK, WILLIAM HINES, MENKA JAIN, BARRETT WELLS, University of Connecticut — Near stoichiometry FeSe films were successfully grown on MgO, SrTiO_{3}, and LaAlO_{3} single crystal substrates using pulsed laser deposition (PLD). X-ray diffraction analysis showed that the FeSe films have a tetragonal structure on SrTiO_{3} and LaAlO_{3} substrates. A mixture of tetragonal and hexagonal structures was observed on MgO substrates due to the larger lattice constant mismatch. The superconductivity of films exhibited a strong dependence on epitaxial strain and thickness. Thicker films (∼ 200 nm) are strained. Films on nearly lattice-matched LaAlO_{3} are superconducting, while films under tension on SrTiO_{3} or MgO are metallic but not superconducting down to 5K. The onset temperature for superconductivity have a near linear magnetic field dependence with dH/dT = -2.8 T/K for fields up to 9T.

1 The work is supported by the US-DOE through contract # DE-FG02-00ER45801.

1:15PM Z35.00011 Crystal growth and superconductivity of new Fe–Te base materials, GENDA GUN, CMP&MS, Brookhaven National Laboratory, NY 11973, USA, JINSHENG WEN, ZHIJUN XU, Z.W. LIN, QIAN Li, J.M. TRANQUADA, CMP&MS, BNL, CMP&MS, BNL TEAM — A number of Fe-base superconducting materials with critical superconducting temperature up to 56K have been discovered recently. Because As and its oxide of the Fe–As base superconducting materials is poison, it is a serious safety issue for researchers to make the bulk materials. The new Fe–Te base superconducting materials with Se doping are less toxic and safe to handle. We have grown a number of the FeTe_{1-x}Se_{x} single crystals (x = 0–0.5) by using a modified floating-zone growth technique. The effects of the growth condition and the composition of a feed rod on the critical superconducting temperature of FeTe_{1-x}Se_{x} have been studied by using a floating zone machine. The single crystals of the PbO-type tetragonal structure FeTe_{1-y}Fe_{y} (y = 0.04 to 0.08) are not superconducting. When Se substitutes for Te in FeTe_{1-x}Se_{x} single crystals, the superconducting transition temperature increases with increasing Se content.

1 This work is supported by DOE under contract No. DE-AC02-98CH10886.
which indicates that this cluster's stability could be accounted for by the Jellium model. The Al$_3$Bi cluster has a large ionization potential of 7.1 eV, a low electron affinity of 1.4 eV and a HOMO-LUMO gap of 1.7 eV. The molecular orbitals of Al$_3$Bi are two very compact structure of Al$_3$Bi, which consist of alternated Fe-X and electron-doping Tl layers, very similar to ternary BaFe$_2$As$_2$ system. As in all the Fe-based superconductors, the electronic structure near the Fermi level is dominated by Fe 3d states, with a pseudogap. Tl occurs with valence Tl$^+_{1}$, and thus provides heavy electron-doping with 0.5 additional carrier per Fe relative to Fe-X layers. This pushes the Fermi level to the upper edge of the pseudogap and results in disappearance of hole cylinders of Fermi surface at zone center. As expected, the spin density wave instability is completely suppressed and the checkerboard antiferromagnetism becomes the favored magnetic order. This over-doped system may be helpful in elucidating the magnetic, superconducting mechanism, and spin pseudogap behavior in Fe-based materials. Ti deficiency is predicted to reinstate the part of hole Fermi surface and again induce spin fluctuations corresponding to the spin density wave, which are essential for pairing states in Fe-based superconductors.

We gratefully acknowledge support from the U. S. Department of the Army through a MURI grant W911NF-06-1-0280.
11:51 AM Z37.00004 Copper nanocluster growth at experimental conditions using temperature accelerated dynamics, C. S. DIAS, GCEP-Centro de Física da Universidade do Minho, Braga, Portugal. T-1 Group, MS B268, Los Alamos National Laboratory, Los Alamos, USA. — We study the dynamics of vapor phase cluster growth near experimental conditions of pressure at temperatures below 200K. To this end, we carried out temperature accelerated dynamics (TAD) simulations at different vapor pressures to characterize the morphology of the resulting nanoparticles, which leads to a range of values of the flux of impinging atoms at fixed vapor temperature. At typical experimental pressures of $10^{-3}$ – $10^{-4}$ bar TAD provides substantial boost over regular Molecular Dynamics (MD). TAD is also advantageous over MD, regarding the sampling of the network of visited states, which provides a deeper understanding of the evolution of the system. We characterize the growth of such clusters at different vapor pressures.

12:03PM Z37.00005 Photoabsorption by Volume Plasmons in Metal Clusters1, CHUNRONG YIN, CHUNLEI XIA, Vitaly Kresin. University of Southern California. Metal clusters exhibit strong photoabsorption resonances in the visible part of the spectrum. These are collective "surface plasmon" excitations which have been extensively investigated. However, the UV part of the spectrum has remained rather unexplored. Some theoretical calculations have predicted that a measurable portion of the delocalized valence electrons' dipole oscillator strength should be located in this region. This predicted absorption feature has been ascribed to a volume-plasmon type of excitation, which in small particles can couple to light, in contradistinction to the situation in bulk metals. We have carried out a photodepletion cross section measurement on a pair of prototypical simple-metal nanoclusters, Na$_{20}$ and Na$_{55}$, finding that these systems indeed possess a broad volume-plasmon absorption peak centered at $\approx 4$ eV and having an oscillator strength contents of $\approx$15-20% of the total, in good agreement with theoretical calculations. These spectra provide the first experimental confirmation of the existence of optically active volume-type collective electronic excitations in metal nanocluster particles.

1Supported by NSF.

12:15PM Z37.00006 Atomic Dipole Moments and Polarizabilities of Na$_N$ Clusters, N= 2-30, 38, and 55, 1, KOBLAR JACKSON, LI MA, Central Michigan University, Mount Pleasant, MI 48859, MINGLI YANG, Institute for Nanobiomedical Technology and Membrane Biology, West-China Medical School/West-China Hospital, Sichuan University, Chengdu, China, JULIUS JELLINEK, Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne IL 60439, USA. — The response of Na$_N$ clusters, N = 2 - 30, 38, and 55 to a static external electric field is studied using a new method that decomposes the total cluster dipole moment and polarizability into contributions from non-overlapping atomic volumes (Jackson et al., J. Chem. Phys. 129, 144309 (2008)). The atomic dipole moments and polarizabilities are in turn partitioned into local dipole and charge-transfer components, corresponding to dielectric and metallic responses, respectively. Analysis of the atomic polarizabilities indicates a strong dependence on the location of the atoms within the clusters and shows directly the effect of electrostatic screening in the clusters. We show that the relative importance of the charge-transfer component of the cluster polarizability increases with cluster size and approaches the bulk-limit on a per-atom basis for clusters as small as 20 atoms. The charge-transfer component is shown to be responsible for the structure/shape driven variations, and for shape-related anisotropies, in the cluster polarizabilities.

1This work was supported by the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, U. S. Department of Energy under grant number DE-FGO2-03ER15489.

12:27PM Z37.00007 Magnetic Properties of Arsenic Cluster Assemblies1, MEICHUN QIAN, A. C. REBER, S. N. KHANNA, Dept. of Physics, Virginia Commonwealth University, A. SEN, S. MANDAL, N. K. CHAKI, Depts. of Chemistry and Physics, Penn. State University. — Clusters have the potential to serve as building blocks of materials, enabling the tailoring of materials with novel properties. Recently, we synthesized a magnetic cluster assembled material using the As$_7$ cluster and cryptated K, which are the elements from main group. X-ray studies show that the As$_7$ cluster is distorted to accompany two cryptated K. We have investigated the magnetic properties of As cluster assembly using density functional theory. We found the As$_7$ cluster has the (-2) valence state and possess one unpaired electron. The magnetic state is stabilized in the crystal and has a lower energy of 90 meV than the nonmagnetic state. The magnetic moments are located on the As$_7$ cluster and display antiferromagnetic order in the crystal. We also study the magnetic properties of the As cluster assemblies with transition metal as a linker, and these findings are possible to provide a new kind of magnetic materials.

1Supports from US AFOSR, ARO and DOE.

12:39PM Z37.00008 Interpreting the magnetic and electric deflections of free metal clusters in molecular beams, ANTHONY LIANG, JOHN BOWLAN, WALTER DE HEER. — A short review of the analysis of magnetic and electric deflection data will be presented. Electric and magnetic beam deflection of several metal clusters, including Au$_N$, Al$_N$, Nb$_N$O, Na$_N$, Ho$_N$, Co$_N$, Rh$_N$ at various temperatures (20K-300K) and field strengths will be presented. The relation between the broadening of the deflected beam and the polarization distribution of the ensemble assuming a classical polar spherical rigid rotor model is demonstrated. Complicating factors including asymmetry effects and residual temperature effects will be discussed.

12:51PM Z37.00009 Comparative study of metal clusters by Quantum Monte Carlo method1, YUNING WU, HAI-PING CHENG, Quantum Theory Project, Department of Physics, University of Florida, PAUL KENT, CNMS, Oak Ridge National Lab — Lithium and sodium clusters have been studied by fixed-node diffusion quantum Monte Carlo method. This stochastic wave-function-based approach can provide more accurate results and serve as benchmarks against which other techniques may be compared. We studied the binding energies and investigate different geometries to decide the ground state. Our results are compared with those derived from other method such as DFT and CI methods. Our objective is to validate current quantum Monte Carlo methods for small metal clusters that undergo size dependent geometrical transitions.

1Acknowledgment: DOE/BES DE-FG02-02ER45995; portion of this work at CNMS at ORNL sponsored by Division of User Facilities, Office of Basic Energy Sciences, US Department of Energy.
modeled using Lennard-Jones potentials. Our results show that the cantilever deflection depend on the combination of the Lennard-Jones parameters as well as surface tension and strain energy. In this work, we use a molecular approach to describe the entire system. In particular, the solid beam is modeled as a collection of biosensors utilizing nano or micro-sized cantilevers. Through chemical coating of probe molecules that exhibit strong affinity to the target molecules, the calculated HOMO-LUMO gap of 1.89 eV, and can be viewed as a gas phase Zintl analogue of Sn.

CASTLEMAN GROUP COLLABORATION — Here we present evidence that the gap between the highest occupied and lowest unoccupied molecular orbitals (XANES), will also be presented to demonstrate the evolution of O vacancies and possible N impurities due to thermal annealing in the IBAD deposited films. Of structural stability, the short-range-order local structural information obtained from EXAFS measurements is of central importance. Powder samples with (EXAFS) technique. These materials have shown cubic long-range-order structure and high hardness without chemical stabilizers. To understand the origin of structural stability, the short-range-order local structural information obtained from EXAFS measurements is of central importance. Powder samples with different nanoparticle sizes prepared by different sol-gel processes were analyzed. Zr k-edge EXAFS, as well as N k-edge x-ray absorption near-edge structures (XANES), will also be presented to demonstrate the evolution of O vacancies and possible N impurities due to thermal annealing in the IBAD deposited films.

TPD over laboratory time scales. Although the simulated TPD spectra agree with experiment, a detailed analysis reveals underlying kinetic phenomena that contrast the standard experimental interpretation and opens new possibilities for understanding molecular kinetics at solid surfaces.

In this work, we use accelerated molecular-dynamics to simulate TPD of pentane from the basal plane of graphite, in the first atomistic simulations to probe TPD over laboratory time scales. Although the simulated TPD spectra agree with experiment, a detailed analysis reveals underlying kinetic phenomena that contrast the standard experimental interpretation and opens new possibilities for understanding molecular kinetics at solid surfaces.

1:03PM Z37.00010 Electronic Structure of Bi₃Ga₃−y Semiconductor Clusters and the Special Stability of Bi₃Ga₃ - A Gas Phase Zintl Analogue; JOSE ULISES REVELES, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284, UJJWAL GUPTA, JOSHUA J. MELKO, Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802, SHIV N. KHANNA, Department of Physics, Virginia Commonwealth University, Richmond VA, 23284, A. W. CASTLEMAN, JR., Departments of Chemistry and Physics, The Pennsylvania State University, University Park, PA 16802, SHIV KHANNA RESEARCH GROUP COLLABORATION, THE CASTLEMAN GROUP COLLABORATION — Here we present evidence that the gap between the highest occupied and lowest unoccupied molecular orbitals (HOMO-LUMO gap) can be tuned (1.12eV-1.89eV) by changing the Ga composition of Bi₃Ga₃ neutral and anionic clusters, some of which display special stability. Collaboratively, mass spectrometry, photoelectron spectroscopy and computational results show that Bi₃Ga₃ is a very stable cluster with a large calculated HOMO-LUMO gap of 1.89 eV, and can be viewed as a gas phase Zintl analogue of Sn⁺², already synthesized in the solution phase. The stability of Bi₃Ga₃ is further attributed to the fact that it has 12 valence electrons and possesses a closo structure in agreement with Wade’s rules.

1:15PM Z37.00011 Simulation of the Adsorption on Nano/Micro-Cantilever Sensors; PADET KHOSATHIT, PHILLIP CHOI, P.-Y. BEN JAR, University of Alberta — Recent advances in nano/micro fabrication techniques have led to the development of biosensors utilizing nano or micro-sized cantilevers. Through chemical coating of probe molecules that exhibit strong affinity to the target molecules, the cantilever would deflect when the target molecules bind with the probe molecules. Previous simulation studies on these systems often involved the use of a multi-scale approach in which molecular models are used for the probe and target molecules while the cantilever is modeled as a continuum solid beam using surface tension and strain energy. In this work, we use a molecular approach to describe the entire system. In particular, the solid beam is modeled as a collection of molecules connected by lattice springs. The intermolecular interactions between the three types of molecules (i.e., probe, target and cantilever molecules) are modeled using Lennard-Jones potentials. Our results show that the cantilever deflection depend on the combination of the Lennard-Jones parameters as well as the number and positions of the probe and target molecules. Details of their effects will be presented in the paper.

1:27PM Z37.00012 Origin of Structural Stability in Cubic ZrO2 Nanocrystals Studied by EXAFS; Y.-L. SOO, S.L. CHANG, National Tsing Hua University, Taiwan, C.L. CHEUNG, R. SABIRIANOV, F. NAMARAV, W.N. MEI, University of Nebraska, P. CHU, National Central University, Taiwan, J.F. LEE, NSRRC, Taiwan — Local environments surrounding Zr nanocrystalline powders and thin films of cubic zirconia prepared by sol-gel and ion beam assisted deposition (IBAD) methods were investigated by using extended x-ray absorption fine structure (EXAFS) technique. These materials have shown cubic long-range-order structure and high hardness without chemical stabilizers. To understand the origin of structural stability, the short-range-order local structural information obtained from EXAFS measurements is of central importance. Powder samples with different nanoparticle sizes prepared by different sol-gel processes were analyzed. Zr k-edge EXAFS, as well as N k-edge x-ray absorption near-edge structures (XANES), will also be presented to demonstrate the evolution of O vacancies and possible N impurities due to thermal annealing in the IBAD deposited films.

This work has been supported by NSC in Taiwan.

Friday, March 20, 2009 11:15AM - 2:15PM –
Session Z38 DCP: Surfaces, Interfaces, and Colloids II 410

11:15AM Z38.00001 Understanding surface energies of transition metals with density-functional theory; ALOYSIUS SOON, MARTIN FUCHS, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG — Determining index-specific surface energies of metals is, to date, still a non-trivial task, both experimentally and theoretically. Density-functional theory (DFT) calculations within the local-density approximation (LDA) for exchange-correlation (XC) have provided understanding of qualitative trends. Yet, absolute surface energies, in particular of d/metals still exhibit significant uncertainties related to the description of XC: gradient-corrected functionals (GGA) which improve over the LDA for other properties often predict less accurate surface energies. This calls for a careful analysis of XC effects on surface energies, including non-local exchange and/or correlation. Here we analyze the surface energies of 4d/metals with modern GGA functionals (PBEsol, AM05, developed to better describe bulk solids and (jellium) surfaces than the LDA and previous GGAs), using the all-electron FHI-aims code [1]. Relating the bulk cohesive energy and surface energy via a bond-cutting model we find modern GGA can indeed correct the poorer results of the usual PBE-GGA but worsen the bulk cohesive energies of 4d/metals. In addition, we consider hybrid XC functionals, using a cluster correction scheme [2], and discuss the effects of including exact exchange on the calculated surface energies.


11:27AM Z38.00002 The initial stages of NaCl dissolution: Ion or ion pair solvation?; JIRI KLIMES, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London — The interaction of water with rock salt (NaCl) is important in a wide variety of natural processes and human activities. A lot is known about NaCl dissolution at the macroscopic level but we do not yet have a detailed atomic scale picture of how salt crystals dissolve. Here we report an extensive series of density functional theory, forcefield and molecular dynamics studies of water clusters at flat and defective NaCl surfaces and NaCl clusters. The focus is on answering seemingly elementary questions such as how many water molecules are needed before it becomes favorable to extract an ion or a pair of ions from the crystal or the cluster. It turns out, however, that the answers to these questions are not so straightforward: below a certain number of water molecules (~12) solvation of individual ions is less costly and above this number solvation of ion pairs is favored. These results reveal a hitherto unknown complexity in the NaCl dissolution process born out of a subtle interplay between water-water and water-ion interactions.

11:39AM Z38.00003 Accelerated Molecular Dynamics of Temperature-Programmed Desorption; KRISTEN FICHTHORN, KELLY BECKER, MARIA MIGNOGNA, Penn State University — The most widely used experimental method for quantifying thermal desorption is temperature-programmed desorption (TPD). Despite its extensive use, interpretation of this experiment can still be controversial. A significant difficulty with interpreting TPD is that this macroscopic experiment offers a limited picture of the underlying microscopic kinetic events. In this work, we use accelerated molecular-dynamics to simulate TPD of n-pentane from the basal plane of graphite, in the first atomistic simulations to probe TPD over laboratory time scales. Although the simulated TPD spectra agree with experiment, a detailed analysis reveals underlying kinetic phenomena that contrast the standard experimental interpretation and opens new possibilities for understanding molecular kinetics at solid surfaces.

This work has been supported by NSF DMR 0514336.
surface potential AFM measurements, however, reveal an apparently anomalous strong dependence of surface potential on the sizes and ratios of $m$.

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### 12:03PM Z38.00005 Probing colloidal physics on the nanometer length scale

**SUNIL SAINIS, Post Doc. Fellow, FRANK VOLLMER, Rowland Junior Fellow** — The sharp spectral features associated with ultra-high Q microresonator modes are sensitive to changes in the local environment and surface of the resonator [1]. Microresonator cavities have been used to detect the binding of single molecules [2] and viruses in an aqueous medium. We report on recent experiments that use microresonators to access colloidal physics on the nanometer length scale. We examine shifts in the resonator as a function of bulk ionic strengths and surface adsorption in a colloid.


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### 12:15PM Z38.00006 Effect of boundary condition on the viscosity of olefins: A molecular dynamics study

**LING TI KONG, COLIN DENNISTON, MARTIN MUSER, University of Western Ontario, YUE QI, General Motor** — The viscosity of hexene was examined by means of non-equilibrium molecular dynamics simulations under different wall-liquid boundary conditions, namely over-smooth wall, more or less realistic wall, and over-adhesive wall. It is found that the wall-liquid interaction plays an important role in the ordering/layering of liquid, and consequently affects the behavior of olefins upon different normal pressures. With the same moving speeds of walls, the shear-rate (the slope of velocity profile) in the liquid is found to decrease with the increasing of normal pressure under over-smooth wall condition, while it is found to increase under the over-adhesive wall condition. The viscosity, in turn, shows a linear dependence on the normal pressure under over-smooth condition while exhibits an exponential dependence under the over-adhesive wall condition. The underlying mechanism of these observations will be presented and discussed in this talk.

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### 12:27PM Z38.00007 Suppressing and Amplifying Depletion Attractions between Surfaces Roughened by Asperities

**KUN ZHAO, THOMAS MASON, UCLA** — Motivated by recent experiments on roughness-controlled depletion attractions, we study the effect of roughness on depletion attractions between flat surfaces decorated using hemispherical and hemispherial asperities. Our calculations show that the depletion attraction between rough surfaces can be either dramatically reduced or amplified depending on the details of the surface morphologies. This model also explains the observed self-assembly of rough Janus platelets into dimers and provides quantitative predictions of roughness-controlled depletion attractions for conditions that have not yet been explored experimentally.

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### 12:39PM Z38.00008 The Dynamics of Charging of Muscovite Mica: Measurement and Modeling

**PAUL J. SIDES, Professor, Carnegie Mellon Univ, DANISH FARUQUI, PhD Student, Carnegie Mellon University, ANDREW J. GELLMAN, Professor, Carnegie Mellon Univ** — The advent of a new method for measuring the zeta potential of planar surfaces, the rotating disk, allowed the investigation of the charging process of mica after immersion in water. The zeta potential of freshly-cleaved muscovite mica was recorded within seconds of immersion of the sample and in fractions of a second thereafter. The zeta potential of mica in water at pH = 5.6 with no added potassium changed by 40 – 50 mV over the charging process of mica after immersion in water. The charging of mica in alkaline KCl solutions of arbitrary concentration, however, was too fast for observation. The charging of mica in alkaline KCl solutions of arbitrary concentration, however, was too fast for observation. The equilibrium zeta potential depended on the logarithm of salt concentration, in agreement with a model based on ion exchange reactions. The average values of the potassium adsorption, proton desorption, potassium adsorption, and potassium desorption rate coefficients were 45 liter/s ± 0.0014/s ± 0.0006, 58 liter/s ± 5, and 0.14/s ± 0.03, respectively. Web Page: http://zetaspin.com

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### 12:51PM Z38.00009 Effects of Embedded Dipoles on the Electrical Response of Self Assembled Monolayers

**P.P. ZHANG, O.M. CABARCOS, T.A. DANIEL, P.S. WEISS, D.L. ALLARA, The Pennsylvania State University** — There has been recent interest in the use of polar molecules assembled at electrodes for tuning work functions and engineering charge injection barriers in organic electronic devices. With this in mind we have been investigating the electrostatic properties of simple model systems prepared from self-assembled alkanethiolate monolayers on Au(111) with the incorporation of an embedded ester moiety [-(CO$_2$)$_{n}$ = $E$] in the adsorbate molecules. The intrinsic static dipole moment of the ester moiety of ~1 Debye magnitude leads to the formation of a strong, highly organized, planar electric dipole layer in the SAM. From our previous X-ray photoelectron spectroscopy data we observe a consistent shift of the C 1s photoelectron kinetic energies between the top and bottom alkyl segments, defined as -(CH$_2$)$_m$ –E-(CH$_2$)$_n$, regardless of the relative lengths $m$ and $n$. This shift correlates well with the value of the electrostatic potential across the E layer. Our recent surface potential AFM measurements, however, reveal an apparently anomalous strong dependence of surface potential on the sizes and ratios of $m$ and $n$, in contrast to the constant electrostatic potential observed in XPS measurements. Mechanisms underlying these effects will be discussed, with possible implications for the electrostatic behavior of more complicated organic and biological systems.

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### 1:03PM Z38.00010 Interfacial Composition of the Ionic Aqueous Solution Studied by the Adsorption of the Cationic Molecules

**JINSUK SONG, MAHN KIM, Physics Department, KAIST** — Knowing the interfacial composition of the ionic aqueous solution is important not only for understanding many atmospheric and environmental chemistry processes 1 but also for understanding many biological processes because the interaction between biomaterials happens often at the interfacial region such as water-vesicle interface in ionic aqueous solution. In this study, the surface anion density is estimated by measuring the surface density and adsorption angle of the cationic molecule, Malachite Green(MG) adsorbed at the air-ionic aqueous solution interface using the second harmonic generation technique. The anion number density at the interface increases with the increasing concentration of the ions and with the increasing size of the anions for spherical ions. It is consistent with other experimental measurements and simulation results2,3. However, it seems that the anion density depends not only on the anion but also on the cation and shape and chemical composition of the ions. 1 E. Knipping et al., Science 288, 301 (2000) 2 S. Ghosal et al., Science 307, 563 (2005) 3 P. Jungwirth et al., J. Phys. Chem. B 105, 10468 (2001)
Coverage Dependent X-ray Photoemission on Halogenated Benzene on Graphite

We studied the adsorption of isomers of halogenated benzene on graphite. We found difference in the behavior of three different symmetry types, (1,2), (1,3), and (1,4), of diiodobenzene (C_6H_4I_2) and 1,4-bromiodobenzene (C_6H_4IBr) adsorbed on graphite surface at 95K by X-ray photoemission spectroscopy. Although the molecules are expected to be similar in their electronic structure, the sticking coefficients and the strength of screening effects are considerably different for the different isomers. We find evidence for different intermolecular interactions both in the initial state and in the final state as well. Symmetry, not simply the chemical constituents, play a role in adsorbate chemistry.

Funded by NSF CHE-0650453

Retardation of ice crystallization by short peptides

The effect of short peptides on the growth of ice crystals is studied using molecular dynamics simulations. The simulations focus on two sequences (Gly-Pro-Ala-Gly and Gly-Gly-Ala-Gly) that are found in collagen hydrolysate, a substance that is known to retard crystal growth. In the absence of peptides, the growth of ice crystal in the solution with the ice/water interface is observed at a rate comparable to the experimental data. When peptides are present in the liquid phase, the crystal growth is retarded to a significant extent compared to the pure water. It is found that Gly-Pro-Ala-Gly is more effective (crystallization is up to 5 times slower than in its absence) than Gly-Gly-Ala-Gly (up to 3 times slower) implying that the role of the proline residue is important. The mechanism can be understood in the nature of binding of the peptides to the growing crystal.

Supported by the United States Department of Agriculture National Research Initiative Program (Grant No. 2006-35503-16998)

AC Electrowetting of Polymer Aqueous Drops on Parallel Electrodes

We have recently observed the strong field dependence of AC-electrowetting of simple electrolyte aqueous drops on parallel gold electrodes, yet the detailed dynamic process of AC-field induced surface wetting remains unclear. In this work, we use fluorescence labeled DNA aqueous solution as a model system to directly visualize the wetting process of aqueous drops under varied AC electric fields by using combined fluorescence microscopy and contact angle goniometer. The electrowetting behavior of DNA aqueous drops is observed at AC-field frequency greater than the reciprocal of the RC time scale for electrode screening. And the onset of AC electrowetting is accompanied by the observed oscillation in drop contour shape and contact line. In addition, the ejection of nanodrops from the parent aqueous drop is observed when the threshold AC-field amplitude is exceeded. A scaling theory based on electrode interfacial screening is developed to quantify the AC-electrowetting behavior with the dependence of AC-field frequency, strength and medium conductivity.

The research is supported by the Petroleum Research Fund, American Chemical Society.

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